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(54) Title: DRUG THERAPY FOR CELIAC SPRUE

(57) Abstract: Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto are decreased by administration of an HLA-binding peptide inhibitor. Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific T cells.



DRUG THERAPY FOR CELIAC SPRUE

CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims priority to U.S. Provisional Application 60/380,761 filed May 14, 2002; to U.S. Provisional Application 60/392,782 filed June 28, 2002; and to U.S. Provisional application no. 60/422,933, filed October 31, 2002, and to U.S. Provisional Application 60/428,033, filed November 20, 2002, each of which are herein specifically incorporated by reference.

BACKGROUND OF THE INVENTION

In 1953, it was first recognized that ingestion of gluten, a common dietary protein present in wheat, barley and rye causes a disease called Celiac Sprue in sensitive individuals. Gluten is a complex mixture of glutamine- and proline-rich gliadin and glutenin molecules and is thought to be responsible for induction of Celiac Sprue. Ingestion of such proteins by sensitive individuals produces flattening of the normally luxurious, rug-like, epithelial lining of the small intestine known to be responsible for efficient and extensive terminal digestion of peptides and other nutrients. Other clinical symptoms of Celiac Sprue include fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, anemia, as well as an enhanced risk for the development of osteoporosis and intestinal malignancies such as lymphoma and carcinoma. The disease has an incidence of approximately 1 in 200 in European populations and is believed to be significantly under diagnosed in other populations.

A related disease is dermatitis herpetiformis, which is a chronic eruption of the skin characterized by clusters of intensely pruritic vesicles, papules, and urticaria-like lesions. IgA deposits occur in almost all normal-appearing and perilesional skin. Asymptomatic gluten-sensitive enteropathy is found in 75 to 90% of patients and in some of their relatives. Onset is usually gradual. Itching and burning are severe, and scratching often obscures the primary lesions with eczematization of nearby skin, leading to an erroneous diagnosis of eczema. Strict adherence to a gluten-free diet for prolonged periods may control the disease in some patients, obviating or reducing the requirement for drug therapy. Dapsone, sulfapyridine, and colchicines are sometimes prescribed for relief of itching.

Celiac Sprue (CS) is generally considered to be an autoimmune disease and the antibodies found in the serum of the patients support the theory that the disease is immunological in nature. Antibodies to tissue transglutaminase (TG2, tTGase or tTG) and gliadin appear in almost 100% of the patients with active CS, and the presence of such antibodies, particularly of the IgA class, has been used in diagnosis of the disease.

[05] The large majority of patients express the HLA-DQ2 [DQ(a1*05, b1*02)] and/or DQ8 [DQ(a1*03, b1*0302)] molecules. It is believed that intestinal damage is caused by interactions between specific gliadin oligopeptides and the HLA-DQ2 or DQ8 antigen, which in turn induce proliferation of T lymphocytes in the sub-epithelial layers. T helper 1 cells and cytokines apparently play a major role in a local inflammatory process leading to villous atrophy of the small intestine.

At the present time, there is no good therapy for the disease, except to avoid completely all foods containing gluten. Although gluten withdrawal has transformed the prognosis for children and substantially improved it for adults, some people still die of the disease, mainly adults who had severe disease at the outset. A leading cause of death is lymphoreticular disease, especially intestinal lymphoma. It is not known whether a glutenfree diet diminishes this risk. Apparent clinical remission is often associated with histologic relapse that is detected only by review biopsies or by increased titers of antibodies to tTGase (also called EMA antibodies).

Gluten is so widely used, for example, in commercial soups, sauces, ice creams, hot dogs, and other foodstuffs, that patients need detailed lists of foodstuffs to avoid and expert advice from a dietitian familiar with celiac disease. Ingesting even small amounts of gluten may prevent remission or induce relapse. Supplementary vitamins, minerals, and hematinics may also be required, depending on deficiency. A few patients respond poorly or not at all to gluten withdrawal, either because the diagnosis is incorrect or because the disease is refractory. In the latter case, oral corticosteroids (e.g., prednisone 10 to 20 mg bid) may induce response.

In view of the serious and widespread nature of Celiac Sprue and the difficulty of removing gluten from the diet, better methods of treatment are of great interest. In particular, there is a need for treatment methods that allow the Celiac Sprue individual to eat gluten-containing foodstuffs without ill effect or at least to tolerate such foodstuffs in small or moderate quantities without inducing relapse. The present invention meets this need for better therapies for Celiac Sprue.

SUMMARY OF THE INVENTION

In one aspect, the present invention provides methods for treating Celiac Sprue and/or dermatitis herpetiformis and the symptoms thereof by administration of an HLA-binding peptide inhibitor to the patient. In one embodiment, the HLA-binding peptide inhibitor employed in the method is an analog of an immunogenic gluten peptide, where an immunogenic gluten peptide is altered by the replacement of one or more amino acids, where the replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like. Analogs of

immunogenic gluten peptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells, are useful agents to treat Celiac Sprue.

[10] In another aspect, the present invention provides novel HLA-binding peptide inhibitors and methods for treating Celiac Sprue and/or dermatitis herpetiformis by administering those compounds.

In another aspect, the invention provides pharmaceutical formulations comprising an HLA-binding peptide inhibitor and a pharmaceutically acceptable carrier. In one embodiment, such formulations comprise an enteric coating that allows delivery of the active agent to the intestine, and the agents are stabilized to resist digestion or acid-catalyzed modification in acidic stomach conditions. In another embodiment, the formulation also comprises one or more glutenases, as described in U.S. Provisional Application 60/392,782 filed June 28, 2002; and U.S. Provisional Application 60/428,033, filed November 20, 2002, both of which are incorporated herein by reference. The invention also provides methods for the administration of enteric formulations of one or more HLA-binding peptide inhibitors to treat Celiac Sprue.

In another aspect, the invention provides methods for screening candidate compounds to determine their suitability for use in the subject methods, by assessing the ability of a candidate agent for its ability to bind to HLA molecules, and/or to inhibit the activity of T cells reactive against gluten antigens.

(extracellular) domain of human HLA-DQ2 bound to an immunodominant gluten epitope, and for identifying molecules that will compete with the gluten peptide for MHC binding. In one embodiment, the methods of the invention utilize structural modeling, and the identification and design of molecules having a particular structure. The structural data provided herein is used for the rational design of drugs that affect immune system activation in Celiac Sprue and/or dermatitis herpetiformis. Analysis of the crystal structure in conjunction with sequence data identifies residues in the immunogenic gluten peptide that are important for interaction with the MHC molecule, and those that are accessible for interaction with the T cell antigen receptor. This information provides a basis for rational drug design.

[14] These and other aspects and embodiments of the invention and methods for making and using the invention are described in more detail in the description of the drawings and the invention, the examples, the claims, and the drawings that follow.

DETAILED DESCRIPTION OF THE EMBODIMENTS

Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides. Therapeutic benefit can be enhanced in some individuals by increasing the digestion of gluten oligopeptides, whether by pretreatment of foodstuffs to be ingested or by administration of an enzyme capable of digesting the gluten oligopeptides, together with administration of an HLA-binding peptide inhibitor. Gluten oligopeptides are highly resistant to cleavage by gastric and pancreatic peptidases such as pepsin, trypsin, chymotrypsin, and the like, and their prolonged presence in the digestive tract can induce an autoimmune response. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto can be decreased by administration of an HLA-binding peptide inhibitor. Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells.

Methods and compositions are provided for the administration of one or more HLA-binding peptide inhibitors to a patient suffering from Celiac Sprue and/or dermatitis herpetiformis. In some embodiments and for some individuals, the methods of the invention remove the requirement that abstention from ingestion of glutens be maintained to keep the disease in remission. The compositions of the invention include formulations of tTGase inhibitors that comprise an enteric coating that allows delivery of the agents to the intestine in an active form; the agents are stabilized to resist digestion or alternative chemical transformations in acidic stomach conditions. In another embodiment, food is pretreated or combined with glutenase, or a glutenase is co-administered (whether in time or in a formulation of the invention) with an HLA-binding peptide inhibitor of the invention.

The subject methods are useful for both prophylactic and therapeutic purposes. Thus, as used herein, the term "treating" is used to refer to both prevention of disease, and treatment of a pre-existing condition. The treatment of ongoing disease, to stabilize or improve the clinical symptoms of the patient, is a particularly important benefit provided by the present invention. Such treatment is desirably performed prior to loss of function in the affected tissues; consequently, the prophylactic therapeutic benefits provided by the invention are also important. Evidence of therapeutic effect may be any diminution in the severity of disease, particularly diminution of the severity of such symptoms as fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, and anemia. Other disease indicia include the presence of antibodies specific for glutens, antibodies specific for tissue transglutaminase, the presence of pro-inflammatory T cells and cytokines, and degradation of the villus structure of the small intestine. Application of the methods and compositions of the invention can result in the improvement of any and all of these disease indicia of Celiac Sprue.

Patients that can benefit from the present invention include both adults and children. Children in particular benefit from prophylactic treatment, as prevention of early exposure to toxic gluten peptides can prevent development of the disease into its more severe forms. Children suitable for prophylaxis in accordance with the methods of the invention can be identified by genetic testing for predisposition, e.g. by HLA typing; by family history, and by other methods known in the art. As is known in the art for other medications, and in accordance with the teachings herein, dosages of the HLA-binding peptide inhibitors of the invention can be adjusted for pediatric use.

Because most proteases and peptidases are unable to hydrolyze the amide bonds of proline residues, the abundance of proline residues in gliadins and related proteins from wheat, rye and barley can constitute a major digestive obstacle for the enzymes involved. This leads to an increased concentration of relatively stable gluten derived oligopeptides in the gut. These stable gluten derived oligopeptides, called "immunogenic oligopeptides" herein, bind to MHC molecules, including HLA HLA-DQ2 or DQ8 molecules, to stimulate an immune response that results in the autoimmune disease aspects of Celiac Sprue. In some cases the enzyme tissue transglutaminase selectively deamidates certain glutamine residues in these peptides, thereby enhancing their potency for the DQ2 ligand binding pocket.

HLA-binding peptide inhibitors of the present invention are analogs of immunogenic gluten oligopeptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells. The inhibitor may comprise oligomers of analogs. Multivalent gluten derived epitopes have markedly enhanced immunogenicity. Consequently, multivalent oligopeptides analogs can also be expected to have increased potency for MHC molecules. In addition, these longer peptides can be more resistant toward intestinal brush border proteolysis.

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An immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least about 8 residues, and may comprise at least about 10 residues; at least about 11 residues, at least about 12 residues, at least about 13 residues, at least about 14 residues, or more, where the term "residue" refers to naturally occurring amino acids, non-naturally occurring amino acids, and amino acid mimetics or derivatives; and where the gluten peptide is altered by the replacement of one or more amino acids. The replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like; and may further be derivitized to further reduce the affinity of these ligands for disease-specific T cell receptors. The sequence of immunogenic gluten oligopeptides can be determined by one of skill in the art. Immunogenic gliadin oligopeptides are peptides derived during normal human digestion of gliadins and related storage proteins as described above, from dietary cereals, e.g. wheat, rye, barley, and the

like. Such oligopeptides act as antigens for T cells in Celiac Sprue. For binding to Class II MHC proteins, immunogenic peptides are usually from about 8 to 20 amino acids in length, more usually from about 10 to 18 amino acids. Such peptides may include PXP motifs, such as the motif PQPQLP. Determination of whether an oligopeptide is immunogenic for a particular patient is readily determined by standard T cell activation and other assays known to those of skill in the art.

Among gluten proteins with potential harmful effect to Celiac Sprue patients are [22] included the storage proteins of wheat, species of which include Triticum aestivum; Triticum aethiopicum; Triticum baeoticum; Triticum militinae; Triticum monococcum; Triticum sinskajae; Triticum timopheevii; Triticum turgidum; Triticum urartu, Triticum vavilovii; Triticum zhukovskvi: etc. A review of the genes encoding wheat storage proteins may be found in Colot (1990) Genet Eng (N Y) 12:225-41. Gliadin is the alcohol-soluble protein fraction of wheat gluten. Gliadins are typically rich in glutamine and proline, particularly in the N-terminal part. For example, the first 100 amino acids of α - and γ -gliadins contain ~35% and ~20% of glutamine and proline residues, respectively. Many wheat gliadins have been characterized, and as there are many strains of wheat and other cereals, it is anticipated that many more sequences will be identified using routine methods of molecular biology. Examples of gliadin sequences include but are not limited to wheat alpha gliadin sequences, for example as provided in Genbank, accession numbers AJ133612; AJ133611; AJ133610; AJ133609; AJ133608; AJ133607; AJ133606; AJ133605; AJ133604; AJ133603; AJ133602; D84341.1; U51307; U51306; U51304; U51303; U50984; and U08287. A sequence of wheat omega gliadin is set forth in Genbank accession number AF280605.

Among the immunogenic gluten oligopeptides that may be modified to generate an HLA-binding peptide inhibitor are included the peptide sequence QLQPFPQPELPYP; the sequence PQPELPY; the sequence PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ and longer peptides containing such sequences or multiple copies of such sequences. Gliadins, secalins and hordeins contain several PQPQLPY sequences or sequences similar thereto rich in Pro-Gln residues that are high-affinity substrates for tTGase. The tTGase catalyzed deamidation of such sequences increases their affinity for HLA-DQ2, the class II MHC allele present in >90% Celiac Sprue patients. Presentation of these deamidated sequences by DQ2 positive antigen presenting cells effectively stimulates proliferation of gliadin-specific T cells from intestinal biopsies of most Celiac Sprue patients, providing evidence for the proposed mechanism of disease progression in Celiac Sprue.

[24] Analog oligopeptides of the invention comprise at least one difference in amino acid sequence from a native gluten peptide, by the replacement of an amino acid with a different

amino acid; a non-naturally occurring amino acid, a peptidomimetics, substituted amino acid, and the like. An L-amino acid from the native peptide may be altered to any other one of the 20 L-amino acids commonly found in proteins, any one of the corresponding D-amino acids, rare amino acids, such as 4-hydroxyproline, and hydroxylysine, or a non-protein amino acid, such as β-alanine, ornithine and homoserine. Also included with the scope of the present invention are amino acids that have been altered by chemical means such as methylation (e.g., α -methylvaline), deamidation, amidation of the C-terminal amino acid by an alkylamine such as ethylamine, ethanolamine, and ethylene diamine, and acylation or methylation of an amino acid side chain function (e.g., acylation of the epsilon amino group of lysine), deimination of arginine to citrulline, isoaspartylation, or phosphorylation on serine, threonine, tyrosine or histidine residues. Importantly, each of these altered amino acids provide a functional handle, e.g. amine, alcohol, aryl halide, and the like, which can be regioselectively derivatized to further reduce the affinity of these ligands for disease-specific T cell receptors. Peptide analogs may be further derivatized with substitutions, including, without limitation, ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group, e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. Such derivatives are encompassed by the term "analog".

The proteolytic stability of gluten oligopeptides can be attributed, at least in part, to the presence of PXP motifs, which are resistant to enzymatic degradation. Preferred analogs of immunogenic gluten oligopeptides will comprise one or more proline residues, and may comprise one or more PXP motifs.

An immunogenic gluten peptide of particular interest is the 33-mer LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPF, which is described in detail in International Patent Application US03/04743, herein specifically incorporated by reference. This peptide is both immunogenic and highly stable to proteases. T cell epitopes present in the 33-mer peptide include, *inter alia*, PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY. In one embodiment of the invention, the immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least one T cell epitope selected from the group consisting of PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY.

The structure of an immunogenic gluten oligopeptide bound to a presenting molecule, e.g. HLA-DQ2; HLA-DQ8; etc. can be determined, e.g. by crystallography, NMR, etc., and used to identify residues in a peptide that are involved in the binding to the MHC molecule, and that are involved in the binding to a T cell antigen receptor. Residues identified as accessible for interacting with the T cell receptor may be modified to decrease

the interaction, e.g. by increasing steric hindrance, altering hydrophilicity or hydrophobicity, etc. Residues identified as involved in interaction with the binding cleft of an MHC molecule may be modified to increase the interaction, e.g. by incorporating amino acids known to interact strongly with the binding cleft.

One inhibitor of interest is an oligopeptide or peptidomimetic that comprises the sequence PXPQPELPY, where X is Gly, Ala, Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp, Glu, or any residue that is substantially bulkier or hydrophilic than Phe. Examples of suitable modifications include ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group (e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. The peptide may comprise modifications that increase binding potency to an MHC molecule, by varying residues that facilitate peptide docking into the binding cleft. Examples of such residues include Gln-4, Glu-6, Leu-7, and Tyr-9 (numbering based on the epitope PFPQPELPY). Each of these residues interacts closely with several residues in the DQ2 binding pocket. By using structure-based molecular design methods, these interactions can be optimized.

[29] Another inhibitor of interest is a oligopeptide or peptidomimetic that comprises the sequence PFPQX₁ELX₂Y, where X₁ and X₂ are independently selected from 4-hydroxy-Pro (either isomer at C-4), 4-amino-Pro (either isomer atC-4), or 3-hydroxy-Pro (either isomer atC-3), and proline, with the proviso that at least one of X₁ and X₂ is a residue other than proline.

[30] Peptides and peptide analogs may be synthesized by standard chemistry techniques, including synthesis by automated procedure. In general, peptide analogs are prepared by solid-phase peptide synthesis methodology which involves coupling each protected amino acid residue to a resin support, preferably a 4-methylbenzhydrylamine resin, by activation with dicyclohexylcarbodiimide to yield a peptide with a C-terminal amide. Alternatively, a chloromethyl resin (Merrifield resin) may be used to yield a peptide with a free carboxylic acid at the C-terminus. After the last residue has been attached, the protected peptide-resin is treated with hydrogen fluoride to cleave the peptide from the resin, as well as deprotect the side chain functional groups. Crude product can be further purified by gel filtration, HPLC, partition chromatography, or ion-exchange chromatography.

[31] The present invention provides crystals and structures of HLA-DQ2 bound to antigen, where the antigen is an immunogenic gluten peptide QLQPFPQPELPYP, which may be referred to for brevity as an "HLA-DQ2/peptide complex". The structures and structural coordinates are useful in structural homology deduction, and in developing and

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screening agents that affect the gluten antigen presentation and immunogenicity. The structure information may be provided in a computer readable form, e.g. as a database of atomic coordinates, or as a three-dimensional model. The structures are useful, for example, in modeling interactions of the HLA molecule with the antigen, effect of inhibitors, etc. The structures are also used to identify molecules that bind to or otherwise interact with structural elements. One aspect of the present invention provides crystals of the HLA-DQ2/peptide complex, which can effectively diffract X-rays for the determination of the atomic coordinates.

The present invention further includes methods of using the structural information provided herein to derive a detailed structure of related peptide binding interactions, particularly other gluten peptides, or analogs and mimetics thereof. Such structural homology determination may utilize modeling, alone or in combination with structure determination.

The present invention provides three-dimensional coordinates for the HLA-DQ2/peptide complex. Such a data set may be provided in computer readable form. Methods of using such coordinates (including in computer readable form) in drug assays and drug screens as exemplified herein, are also part of the present invention. In a particular embodiment of this type, the coordinates contained in the data set can be used to identify potential modulators of the HLA-DQ2/peptide complex, including molecules that mimic the binding of the peptide to the HLA molecule, but which lack, or are substantially diminished in the ability to stimulate a T cell response.

In one embodiment, a potential agent for modulation of HLA-DQ2/peptide complex is selected by performing rational drug design with the three-dimensional coordinates determined for the crystal structures. Preferably the selection is performed in conjunction with computer modeling. Rational design may also be used in the genetic modification of immunogenic peptides by modeling the potential effect of a change in the amino acid sequence.

[35] Computer analysis may be performed with one or more of the computer programs including: GRASP, O (Jones et al. (1991) Acta Cryst. A47:110); QUANTA, CHARMM, INSIGHT, SYBYL, MACROMODEL; ICM, and CNS (Brunger et al. (1998) Acta Cryst. D54:905). In a further embodiment of this aspect of the invention, an initial drug screening assay is performed using the three-dimensional structure so obtained, preferably along with a docking computer program. Such computer modeling can be performed with one or more Docking programs such as DOC, GRAM and AUTO DOCK. See, for example, Dunbrack et al. (1997) Folding & Design 2:27-42.

[36] It should be understood that in the drug screening and protein modification assays provided herein, a number of iterative cycles of any or all of the steps may be performed to

optimize the selection. For example, assays and drug screens that monitor the activity of the T cells in the presence and/or absence of a potential inhibitor are also included in the present invention and can be employed as an assay or drug screen, usually as a single step in a multi-step protocol.

The structure of the HLA-DQ2/peptide complex is useful in the design of agents that mimic the activity and/or specificity of the binding interaction. The structures encoded by the data may be computationally evaluated for an ability to associate with chemical entities. This provides insight into an element's ability to associate with chemical entities. Chemical entities that are capable of associating with these domains may alter immunogenicity. Such chemical entities are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a graphical format. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

In one embodiment of the invention, an invention is provided for evaluating the ability of a chemical entity to associate with any of the molecules or molecular complexes set forth above. This method comprises the steps of employing computational means to perform a fitting operation between the chemical entity and the interacting surface of the polypeptide or nucleic acid; and analyzing the results of the fitting operation to quantify the association. The term "chemical entity", as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes. Molecular design techniques are used to design and select chemical entities, including inhibitory compounds, capable of binding to the HLA molecule, or to the gluten peptide. Such chemical entities may interact directly with certain key features of the structure.

It will be understood by those skilled in the art that not all of the atoms present in a significant contact residue need be present in a competitive binding agent. In fact, it is only those few atoms that shape the loops and actually form important contacts that are likely to be important for activity. Those skilled in the art will be able to identify these important atoms based on the structure model of the invention, which can be constructed using the structural data herein.

The design of compounds that bind to HLA-DQ2 according to this invention generally involves consideration of two factors. First, the compound must be capable of either competing for binding with an immunogenic gluten peptide; or physically and structurally associating with the HLA-DQ2 domains. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

[41] The compound must be able to assume a conformation that allows it to interact with the binding pocket. Although certain portions of the compound will not directly participate in

these associations, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of an entity comprising several interacting chemical moleties.

Computer-based methods of analysis fall into two broad classes: database methods [42] and de novo design methods. In database methods the compound of interest is compared to all compounds present in a database of chemical structures and compounds whose structure is in some way similar to the compound of interest are identified. The structures in the database are based on either experimental data, generated by NMR or x-ray crystallography, or modeled three-dimensional structures based on two-dimensional data. In de novo design methods, models of compounds whose structure is in some way similar to the compound of interest are generated by a computer program using information derived from known structures, e.g. data generated by x-ray crystallography and/or theoretical rules. Such design methods can build a compound having a desired structure in either an atomby-atom manner or by assembling stored small molecular fragments. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within the interacting surface of the RNA. Docking may be accomplished using software such as Quanta (Molecular Simulations, San Diego, CA) and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

[43] Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include: SmoG, GRID (Goodford (1985) J. Med. Chem., 28, pp. 849-857; Oxford University, Oxford, UK; MCSS (Miranker et al. (1991) Proteins: Structure, Function and Genetics, 11, pp. 29-34; Molecular Simulations, San Diego, CA); AUTODOCK (Goodsell et al., (1990) Proteins: Structure, Function, and Genetics, 8, pp. 195-202; Scripps Research Institute, La Jolla, Calif.); and DOCK (Kuntz et al. (1982) J. Mol. Biol., 161:269-288; University of California, San Francisco, Calif.)

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates. Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett et al. (1989) In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196; University of California, Berkeley, Calif.); 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif); and HOOK (available from Molecular Simulations, San Diego, CA).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., N. C. Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990). See also, M. A. Navia et al., "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once the binding entity has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit by the same computer methods described above.

Another approach made possible and enabled by this invention, is the computational screening of small molecule databases. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy. Generally the tighter the fit, the lower the steric hindrances, and the greater the attractive forces, the more potent the potential modulator since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug the more likely that the drug will not interact as well with other proteins. This will minimize potential side effects due to unwanted interactions with other proteins.

Compounds of interest can be systematically modified by computer modeling programs until one or more promising potential analogs are identified. In addition systematic modification of selected analogs can then be systematically modified by computer modeling programs until one or more potential analogs are identified. Alternatively a potential modulator could be obtained by initially screening a random peptide library, for example one produced by recombinant bacteriophage. A peptide selected in this manner would then be systematically modified by computer modeling programs as described above, and then treated analogously to a structural analog.

Once a potential modulator/inhibitor is identified it can be either selected from a library of chemicals as are commercially available from most large chemical companies including Merck, GlaxoWelcome, Bristol Meyers Squib, Monsanto/Searle, Eli Lilly, Novartis and Pharmacia UpJohn, or alternatively the potential modulator may be synthesized de novo. The de novo synthesis of one or even a relatively small group of specific compounds is reasonable in the art of drug design.

[50] The success of both database and *de novo* methods in identifying compounds with activities similar to the compound of interest depends on the identification of the functionally

relevant portion of the compound of interest. For drugs, the functionally relevant portion may be referred to as a pharmacophore, *i.e.* an arrangement of structural features and functional groups important for biological activity. Not all identified compounds having the desired pharmacophore will act as a modulator of inflammation. The actual activity can be finally determined only by measuring the activity of the compound in relevant biological assays. However, the methods of the invention are extremely valuable because they can be used to greatly reduce the number of compounds that must be tested to identify an actual inhibitor.

In order to determine the biological activity of a candidate pharmacophore it is preferable to measure biological activity at several concentrations of candidate compound. The activity at a given concentration of candidate compound can be tested in a number of ways.

[52] For example, an HLA molecule can be attached to a solid support. Methods for placing proteins on a solid support are well known in the art and include such steps as linking biotin to the protein, and linking avidin to the solid support. The solid support can be washed to remove unreacted species. A solution of a labeled candidate agent can be contacted with the solid support. The solid support is washed again to remove the potential modulator not bound to the support. The amount of labeled potential modulator remaining with the solid support and thereby bound to the protein can be determined. Alternatively, or in addition, the dissociation constant between the labeled candidate agent and the protein can be determined.

Crystals of the binding complex of the present invention can be grown by a number of techniques including batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and by microdialysis. Seeding of the crystals in some instances is required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used. The crystals may be shrunk by transfer into solutions of different composition, e.g. by the addition of metal ions such as Mn²⁺, Pb²⁺, etc. Crystals may also be generated that include cofactors, substrates, candidate inhibitors, and the like, that interact with the protein, e.g. by cocrystallization of soaking protein crystals in a solution comprising an inhibitor or other agent.

[54] Alternative methods may also be used. For example, crystals can be characterized by using X-rays produced in a conventional source (such as a sealed tube or a rotating anode) or using a synchrotron source. Methods of characterization include, but are not limited to, precision photography, oscillation photography and diffractometer data collection. Selenium-methionine may be used as described in the examples provided herein, or alternatively a heavy metal derivative data set (e.g., using PCMB) may be used in place of the selenium-methionine derivatization.

Electron density maps may be built from crystals using phase information from multiple isomorphous heavy-atom derivatives, molecular replacement or selenomethionine incorporated multiwavelength anomalous disperson technique. Model building is facilitated by the use of sequence markers, especially selenomethionine residues. Anomalous difference Fourier maps may be calculated with data from selenomethionine-substituted HLA-DQ2/ GLUTEN EPITOPE and with experimental multiple isomorphous replacement with anomalous scattering (MIRAS) phases (Hemming and Edwards (2000) J. Biol. Chem. 275:2288). Maps are improved by phase combination, where MIRAS phases are combined by the program SIGMAA (Jones et al., supra.) Phase combination may be followed by solvent flattening with DM (Carson (1997) Methods Enzymol. 277:493). Improved maps may be obtained by combination of the MIRAS phases with improved phases from combined polyalanine and atomic models in an iterative process. The model can be refined by classical positional and B-factor minimization, and with manual rebuilding.

[56] HLA-DQ2/peptide complex structure models and databases of structure information are provided. The structural models find use in determining the structure of related and/or analogous peptide complexes. In some cases, modeling will be based on the provided structure. In other embodiments, modeling will utilize the provided structure in combination with features present in homologous and/or related structures, where relationship may be defined by protein sequence similarity, or structural similarity, e.g. in the presence of specific features as described above.

The structure model may be implemented in hardware or software, or a combination of both. For most purposes, in order to use the structure coordinates generated for the structure, it is necessary to convert them into a three-dimensional shape. This is achieved through the use of free or commercially available software that is capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structure coordinates.

In one embodiment of the invention, a machine-readable storage medium is provided, the medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of any of the structures of this invention that have been described above. Specifically, the computer-readable storage medium is capable of displaying a graphical three-dimensional representation of the HLA-DQ2/peptide complex.

[59] Thus, in accordance with the present invention, data providing structural coordinates, alone or in combination with software capable of displaying the resulting three dimensional structure of the complex, portions thereof, and their structurally similar analogs, is stored in a machine-readable storage medium. Such data may be used for a variety of

purposes, such as drug discovery, analysis of interactions between cellular components during translation, modeling of vaccines, and the like.

Preferably, the invention is implemented in computer programs executing on programmable computers, comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

[61] Each program is preferably implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

[62] Each such computer program is preferably stored on a storage media or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

The HLA-binding peptide inhibitors are incorporated into a variety of formulations for therapeutic administration. In one aspect, the agents are formulated into pharmaceutical compositions by combination with appropriate, pharmaceutically acceptable carriers or diluents, and may be formulated into preparations in solid, semi-solid, liquid or gaseous forms, such as tablets, capsules, powders, granules, ointments, solutions, suppositories, injections, inhalants, gels, microspheres, and aerosols. As such, administration can be achieved in various ways, usually by oral administration. The HLA-binding peptide inhibitors may be systemic after administration or may be localized by virtue of the formulation, or by the use of an implant that acts to retain the active dose at the site of implantation.

In pharmaceutical dosage forms, the HLA-binding peptide inhibitors may be administered in the form of their pharmaceutically acceptable salts, or they may also be used alone or in appropriate association, as well as in combination with other pharmaceutically active compounds. The agents may be combined, as previously described, to provide a cocktail of activities. The following methods and excipients are merely exemplary and are in no way limiting.

[65] For oral preparations, the agents can be used alone or in combination with appropriate additives to make tablets, powders, granules or capsules, for example, with conventional additives, such as lactose, mannitol, corn starch or potato starch; with binders, such as crystalline cellulose, cellulose derivatives, acacia, com starch or gelatins; with disintegrators, such as corn starch, potato starch or sodium carboxymethylcellulose; with lubricants, such as talc or magnesium stearate; and if desired, with diluents, buffering agents, moistening agents, preservatives and flavoring agents.

In one embodiment of the invention, the oral formulations comprise enteric coatings, so that the active agent is delivered to the intestinal tract. Enteric formulations are often used to protect an active ingredient from the strongly acid contents of the stomach. Such formulations are created by coating a solid dosage form with a film of a polymer that is insoluble in acid environments, and soluble in basic environments. Exemplary films are cellulose acetate phthalate, polyvinyl acetate phthalate, hydroxypropyl methylcellulose phthalate and hydroxypropyl methylcellulose acetate succinate, methacrylate copolymers, and cellulose acetate phthalate.

Other enteric formulation comprise engineered polymer microspheres made of biologically erodable polymers, which display strong adhesive interactions with gastrointestinal mucus and cellular linings, can traverse both the mucosal absorptive epithelium and the follicle-associated epithelium covering the lymphoid tissue of Peyer's patches. The polymers maintain contact with intestinal epithelium for extended periods of time and actually penetrate it, through and between cells. See, for example, Mathiowitz et al. (1997) Nature 386 (6623): 410-414. Drug delivery systems can also utilize a core of superporous hydrogels (SPH) and SPH composite (SPHC), as described by Dorkoosh et al. (2001) J Control Release 71(3):307-18.

[68] Formulations are typically provided in a unit dosage form, where the term "unit dosage form," refers to physically discrete units suitable as unitary dosages for human subjects, each unit containing a predetermined quantity of glutenase calculated in an amount sufficient to produce the desired effect in association with a pharmaceutically acceptable diluent, carrier or vehicle. The specifications for the unit dosage forms of the present invention depend on the particular complex employed and the effect to be achieved, and the pharmacodynamics associated with each complex in the host.

The pharmaceutically acceptable excipients, such as vehicles, adjuvants, carriers or diluents, are readily available to the public. Moreover, pharmaceutically acceptable auxiliary substances, such as pH adjusting and buffering agents, tonicity adjusting agents, stabilizers, wetting agents and the like, are readily available to the public.

METHODS OF TREATMENT

The subject methods are used to treat individuals suffering from Celiac Sprue and/or dermatitis herpetiformis, by administering an effective dose through a pharmaceutical formulation. Diagnosis of suitable patients may utilize a variety of criteria known to those of skill in the art. A quantitative increase in antibodies specific for gliadin, and/or tissue transglutaminase is indicative of the disease. Family histories and the presence of the HLA alleles HLA-DQ2 [DQ(a1*05, b1*02)] and/or DQ8 [DQ(a1*03, b1*0302)] are indicative of a susceptibility to the disease. Specific peptide analogs may be administered therapeutically to decrease inflammation, and/or to induce antigen-specific tolerance to treat autoimmunity. Methods for the delivery of peptides that are altered from a native peptide are known in the art. Alteration of native peptides with selective changes of crucial residues can induce unresponsiveness or change the responsiveness of antigen-specific autoreactive T cells.

[71] The therapeutic effect may be measured in terms of clinical outcome, or may rely on immunological or biochemical tests. Suppression of the deleterious T-cell activity can be measured by enumeration of reactive Th1 cells, by quantitating the release of cytokines at the sites of lesions, or using other assays for the presence of autoimmune T cells known in the art. Alternatively, one may look for a reduction in symptoms of a disease.

Various methods for administration may be employed. The dosage of the therapeutic formulation will vary widely, depending upon the nature of the disease, the frequency of administration, the manner of administration, the clearance of the agent from the host, and the like. Such treatment could either be before meals or on a once-a-day basis or on a once-a-week basis, depending on the half-life of the inhibitor. A typical dose is at least about 1 μg, usually at least about 10 μg, more usually at least about 0.1 mg, and not more than about 10 mg, usually not more than about 1 mg. Enteric coating of these peptides may also enhance their lifetimes in the gut, thereby permitting delivery to the proximal and distal small intestinal tissue. Treatment of other autoimmune disorders such as Type I diabetes with such ligands may involve oral, intravenous or intramuscular administration. The initial dose may be larger, followed by smaller maintenance doses. The dose may be administered as infrequently as weekly or biweekly, or more often fractionated into smaller doses and administered daily, with meals, semi-weekly, *etc.* to maintain an effective dosage level.

The HLA-binding peptide inhibitors of the invention may be administered in the treatment of Type 1 diabetes (IDDM). IDDM and celiac disease are both immunologic disorders where specific HLA alleles are associated with disease risk. Transglutaminase autoantibodies can be found in some patients with IDDM. The prevalence of transglutaminase autoantibodies is higher in diabetic patients with HLA DQ2 or DQ8.

Human type I or insulin-dependent diabetes mellitus (IDDM) is characterized by autoimmune destruction of the β cells in the pancreatic islets of Langerhans. The depletion of β cells results in an inability to regulate levels of glucose in the blood. Overt diabetes occurs when the level of glucose in the blood rises above a specific level, usually about 250 mg/dl. In humans a long presymptomatic period precedes the onset of diabetes. During this period there is a gradual loss of pancreatic beta cell function. IDDM is currently treated by monitoring blood glucose levels to guide injection, or pump-based delivery, of recombinant insulin. Diet and exercise regimens contribute to achieving adequate blood glucose control. The inhibitors of the invention may be administered alone, or in combination with other therapies. The route of administration may be oral, as described for treatment of Celiac Sprue, or may be injected, e.g. i.v., i.m., etc. Administration may be performed during the pre-symptomatic phase, or in overt diabetes.

EXPERIMENTAL

Example

It has long been known that the principal toxic components of wheat gluten are a family of closely related Pro-Gln rich proteins called gliadins. Recent reports have suggested that peptides from a short segment of α-gliadin appear to account for most of the gluten-specific recognition by CD4+ T cells from Celiac Sprue patients. These peptides are substrates of tissue transglutaminase (tTGase), the primary auto-antigen in Celiac Sprue, and the products of this enzymatic reaction bind to the class II HLA DQ2 molecule. This "immunodominant" region of α-gliadin is part of an unusually long proteolytic product generated by the digestive process that: (a) is exceptionally resistant to further breakdown by gastric, pancreatic and intestinal brush border proteases; (b) is the highest specificity substrate of human tissue transglutaminase (tTGase) discovered to date; (c) contains at least six overlapping copies of epitopes known to be recognized by patient derived T cells; (d) stimulates representative T cell clones that recognize these epitopes with submicromolar efficacy; and (e) has homologs in proteins from all toxic foodgrains but no homologs in non-toxic foodgrain proteins.

Identification of stable peptides from gastric protease, pancreatic protease and brush border membrane peptidase catalyzed digestion of recombinant α2-gliadin: α2-gliadin, a representative α-gliadin (Arentz-Hansen et al. (2000) Gut 46:46), was expressed in recombinant form and purified from E. coli. The α2-gliadin gene was cloned in pET28a plasmid (Novagen) and transformed into the expression host BL21(DE3) (Novagen). The transformed cells were grown in 1-liter cultures of LB media containing 50 μg/ml of

kanamycin at 37 $^{\circ}$ C until the OD600 0.6-1 was achieved. The expression of α 2-gliadin protein was induced with the addition of 0.4 mM isopropyl α-D-thiogalactoside (Sigma) and the cultures were further incubated at 37 °C for 20 hours. The cells expressing the recombinant α2-gliadin were centrifuged at 3600 rpm for 30 minutes. The pellet was resuspended in 15 ml of disruption buffer (200 mM sodium phosphate; 200 mM NaCl; 2.5 mM DTT: 1.5 mM benzamidine; 2.5 mM EDTA; 2 mg/L pepstatin; 2 mg/L leupeptin; 30% v/v glycerol) and lysed by sonication (1 minute; output control set to 6). After centrifugation at 45000g for 45 min, the supernatant was discarded and the pellet containing gliadin protein was resuspended in 50 ml of 7M urea in 50 mM Tris (pH = 8.0). The suspension was again centrifuged at 45000g for 45 min and the supernatant was harvested for purification. The supernatant containing α2-gliadin was incubated with 1 ml of nickel-nitrilotriacetic acid resin (Ni-NTA; Qiagen) overnight and then batch-loaded on a column with 2 ml of Ni-NTA. The column was washed with 7M urea in 50 mM Tris (pH = 8.0) and α 2-gliadin was eluted with 200 mM imidazole, 7 M urea in 50 mM Tris (pH = 4.5). The fractions containing α 2-gliadin were pooled into a final concentration of 70% ethanol solution and two volumes of 1.5M NaCl were added to precipitate the protein. The solution was incubated at 4 °C overnight and the final precipitate was collected by centrifugation at 45000 g for 30 min, rinsed in water, and re-centrifuged to remove the urea. The final purification step of the α-2 gliadin was developed with reverse-phase HPLC. The Ni-NTA purified protein fractions were pooled in 7 M urea buffer and injected to a Vydac (Hesperia, CA) polystyrene reversephase column (i.d. 4.6 mm × 25 cm) with the starting solvent (30% of solvent B: 1:1 HPLCgrade acetonitrile/isopropanol: 0.1% TFA). Solvent A was an aqueous solution with 0.1% TFA. The separation gradient extended from 30-100% of solvent B over 120 min at a flow rate of 0.8 ml/min.

Table 2, Amount of Peptides Digested after 15 hours

	33-mer	Control A	Control B
H1P0	<20%	>90%	>90%
H2P0	<20%	>61%	>85%
H3P0	<20%	>87%	>95%
H4P0	<20%	>96%	>95%
H5P0	<20%	>96%	>95%

The purity of the recombinant gliadin was >95%, which allowed for facile identification and assignment of proteolytic products by LC-MS/MS/UV. Although many previous studies utilized pepsin/trypsin treated gliadins, it was found that, among gastric and pancreatic proteases, chymotrypsin played a major role in the breakdown of α2-gliadin,

To establish the physiological relevance of this peptide, composite gastric/pancreatic enzymatic digestion of α2 gliadin was then examined. As expected, enzymatic digestion with pepsin (1:100 w/w ratio), trypsin (1:100), chymotrypsin (1:100), elastase (1:500) and carboxypeptidase (1:100) was quite efficient, leaving behind only a few peptides longer than 9 residues (the minimum size for a peptide to show class II MHC mediated antigenicity). In addition to the above-mentioned 33-mer, the peptide WQIPEQSR was also identified, and was used as a control in many of the following studies.

[79]

Example 2

The 33-mer gliadin peptide is an excellent substrate for tTGase, and the resulting product is a highly potent activator of patient-derived T cells: A number of recent studies have demonstrated that regiospecific deamidation of immunogenic gliadin peptides by tTGase increases their affinity for HLA-DQ2 as well as the potency with which they activate patient-derived gluten-specific T cells. It has been shown the specificity of tTGase for certain short antigenic peptides derived from gliadin is higher than its specificity toward its physiological target site in fibronectin, for example, the specificity of tTGase for the α -gliadin

derived peptide PQPQLPYPQPQLPY is 5-fold higher than that for its target peptide sequence in fibrinogen, its natural substrate. The kinetics and regiospecificity of deamidation of the 33-mer α -gliadin peptide identified as above were therefore measured. The k_{cat}/K_M was higher than that reported for any peptide studied thus far: kcat / KM = 440 min-1mM-1 for LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQLPYPQPQPQLPYPQPQPQLPYPQPQPQLP

Structural characteristics of the 33-mer gliadin peptide and its naturally occurring [81] homologs: Sequence alignment searches using BLASTP in all non-redundant protein databases revealed several homologs (E-value < 0.001) of the 33-mer gliadin peptide. Interestingly, foodgrain derived homologs were only found in gliadins (from wheat), hordeins (from barley) and secalins (from rye), all of which have been proven to be toxic to Celiac patients (Figure 7). Nontoxic foodgrain proteins, such as avenins (in oats), rice and maize, do not contain homologous sequences to the 33-mer gliadin. In contrast, a BLASTP search with the entire α2-gliadin sequence identified foodgrain protein homologs from both toxic and nontoxic proteins. Based on available information regarding the substrate specificities of gastric, pancreatic and BBM proteases and peptidases, it is predicted that, although most gluten homologs to the 33-mer gliadin peptide contained multiple proteolytic sites and are therefore unlikely to be completely stable toward digestion, several sequences from wheat, rye and barley are expected to be comparably resistant to gastric and intestinal proteolysis. The stable peptide homologs to the 33-mer α 2-gliadin peptide are OPOPFPPQLPYPQTQPFPPQQPYPQPQPQPQPQQPQQPQQPQqqq (from α 1- and α 6-gliadins); QQQPFPQQPIPQQPQPYPQQPQPYPQQPFPPQQPF (from B1 hordein); QPFPQPQQTFPQQPQLPFPQQPQQPFPQPQ (from y-gliadin); VQWPQQQPVPQPHQPF (from γ -gliadin), VQGQGIIQPQQPAQ (from γ -gliadin), FLQPQQPFPQQPQQPYPQQPQQPFPQ (from γ-gliadin), FSQPQQQFPQPQQPQQSFPQQQPP (from γ-gliadin), QPFPQPQQPTPIQPQQPFPQRPQQPFPQPQ (from ω-secalin). These stable peptides are all located at the N-terminal region of the corresponding proteins. The presence of proline residues after otherwise cleavable residues in these peptides would contribute to their proteolytic stability.

The unique primary sequence of the 33-mer gliadin peptide also had homologs among a few non-gluten proteins. Among the strongest homologs were internal sequences from pertactin (a highly immunogenic protein from *Bordetella pertussis*) and a mammalian inositol-polyphosphate 5-phosphatase of unknown function. In both cases available information suggested that the homology could have biologically relevance. For example, the region of pertactin that is homologous to the 33-mer gliadin peptide is known to be part of the immunodominant segment of the protein. In the case of the homologous phosphatase, the corresponding peptide region of the phosphatase is known to be responsible for vesicular trafficking of the phosphatase to the cytoplasmic Golgi. In analogy with the current picture of how gliadin peptides are presented to HLA-DQ2 via a tTGase mediated pathway, these Pro-Gln-rich segments of both pertactin and the phosphatase are likely to be good tTGase substrates.

Example 3

[83] X-ray Crystallographic Analysis of soluble HLA-DQ2. The soluble extracellular domains of the α - and β -chains of HLA-DQ2 were co-expressed in insect cells using a baculovirus expression system (pAcAB3 vector, BD Biosciences). The DNA sequence of the engineered α - and β -chains is provided in SEQ ID NO:1 and SEQ ID NO:2. The β -chain is fused to a sequence encoding the epitope QLQPFPQPELPY at its N-terminal end, and to a biotin recognition sequence at its C-terminal end. Both subunits are also fused to complementary leucine zipper sequences at their C-terminal ends. Since a Factor Xa proteolysis site is engineered between the leucine zipper sequences and the DQ2 subunits, prior to crystallization the leucine zippers were removed from DQ2 by Factor Xa digestion.

Initial purification of the DQ2 heterodimer from the culture medium was performed on an immunoaffinity column containing an anti-DQ2 monoclonal antibody (2.12.E11) bound to a Protein A Sepharose CL-4B column. Subsequently DQ2 was treated with Factor Xa, and purified from the digestion mixture by anion-exchange chromatography followed by size-exclusion chromatography, and concentrated to 4 mg/ml in 25 mM Tris-HCl, pH 8.0. Crystals of the DQ2-epitope complex were obtained using the hanging drop method. Typically, 2 μL of protein solution (2~4 mg/ml DQ2, 25 mM Tris-HCl, pH 8.0) and 2 μL of precipitant buffer (200 mM ammonium acetate, 40 mM ammonium sulfate, 4% ethylene glycol, 22~26% PEG 3350) were combined in a single drop hanging over 1 mL of precipitant buffer at room temperature. Small crystals appeared within three days and grew to full size in two weeks.

[85] For data collection, crystals were transferred to a cryoprotectant solution (mother liquor containing 28% ethylene glycol) for 2 hours, and then flash cooled at 100K in liquid nitrogen. X-ray diffraction data were collected from a single crystal to 2.22 Å resolution at

beamline 11-1 of the Stanford Synchrotron Radiation Laboratory using a Quantum 315 CCD detector. Oscillation images were processed with DENZO and data reduction was carried out with SCALEPACK.

The structure of DQ2-epitope complex was determined by molecular replacement using the program AMoRe in the CCP4 suite of programs. The 2.4 Å resolution structure of insulin peptide-HLA-DQ8 complex (RCSB accession code: 1JK8) minus the insulin peptide and solvent molecules was used as the search model. After initial refinement with the maximum likelihood function of program REFMAC, iterative cycles of refinement including simulated annealing, temperature factor refinement, and energy minimization were made with the program CNS. Model building and correction were performed using σ_A -weighted F_o - F_c and $2F_o$ - F_c electron density maps with the program O. The current model has R-factor of 0.2209 with a $R_{\rm free}$ of 0.2793 at 2.22 Å resolution. Analysis of the Ramachandran plot generated using the program PROCHECK shows that 91.2 % of residues are in most favored regions, 7.9 % are in additional allowed regions, 0.5 % are in generously allowed regions, and 0.5 % are in disallowed regions.

[87] There are two molecules of DQ2-epitope in the asymmetric unit. In the first complex, α-chain of DQ2, β-chain of DQ2, and the alpha-I epitope peptide (sequence QLQPFPQPELPY) are designated A, B, and C respectively. In the second complex, α-chain, β-chain, and epitope peptide are designated D, E, and F respectively. The model includes 354 water molecules (name: HOH) and 4 ethylene glycol molecules (name: EDO).

Thr-106—His-112 region in chain B and Arg-105—His-112 region in chain E are disordered and thus absent from the model. Superposition of the DQ8 structure suggests that these regions form an extended loop. Side chain conformation of the following residues are undefined due to weak electron density in the corresponding region and therefore only their backbone atoms are included in the model: Asp-135 (in chain B), Leu-2, Gln-3, Tyr-12 (in chain C), Asp-135, Gln-136 (in chain E), and Leu-2, Gln-3 (in chain F).

[89] Structure-based design of DQ2 binding peptide inhibitors. The crystal structure of the DQ2-epitope complex reveals precisely which atoms in the peptide QLQPFPQPELPYP point outward (by inference into the T cell receptor binding pocket). Substitutions at these atoms can yield altered peptide ligands that retain the ability to bind tightly to DQ2 but are no longer able to allow docking of the DQ2-peptide complex into disease specific T cell receptors.

The coordinate of the structure are as follows:

[88]

[90]

Coordinates

REMARK peptide link removed (applied DPEP): from B 105 to B 113
REMARK peptide link removed (applied DPEP): from E 104 to E 113
REMARK disulphide added: from A 107 to A 163
REMARK disulphide added: from B 15 to B 79
REMARK disulphide added: from B 117 to B 173

REMARK	disulp	hide	add	ed:	from	D	107	to D	163		
REMARK	-						15	to E	79		
REMARK	_						117	to E	173		
REMARK REMARK		-		13	3:00:	06	C	reated by	y user:	Kim	
ATOM	1		VAL .	A	2		31.060	3.851	4.095	1.00 39.43	A
ATOM	2	CG1	VAL .	A	2		30.078	2.835	3.531	1.00 40.06	A
ATOM	3	CG2	VAL .	A	2		30.370	5.185	4.344	1.00 39.97	A
ATOM	4	C	VAL.		2		30.653	3.406	6.542	1.00 36.80	A
ATOM	5	0	VAL		2		29.644	2.702	6.527	1.00 38.25	A
ATOM	6	N	VAL		2		32.189	1.926	5.235	1.00 36.80	A
MOTA MOTA	7 8	CA	VAL		2 3		31.684 30.910	3.321 4.267	5.414 7.523	1.00 37.95 1.00 34.99	A A
ATOM	9	n Ca	ALA ALA		3		30.003	4.416	8.658	1.00 32.94	A
MOTA	10	СВ	ALA		3		30.325	3.368	9.721	1.00 33.34	A
MOTA	11	c	ALA		3		30.094	5.805	9.263	1.00 30.81	A
MOTA	12	0	ALA		3		30.980	6.583	8.914	1.00 29.57	A
MOTA	13	N	ASP	A	4		29.172	6.115	10.170	1.00 28.70	A
MOTA	14	CA	ASP	A	4		29.173	7.416	10.822	1.00 26.95	A
MOTA	15	CB	ASP		4		27.812	7.722	11.456	1.00 28.65	A
MOTA	16	CG	ASP		4		26.687	7.845	10.431	1.00 31.67	A
MOTA	17		ASP		4		26.904	8.417	9.339 10.735	1.00 33.31 1.00 33.31	A A
MOTA	18 19	C C	ASP ASP		4 4		25.568 30.254	7.381 7.432	11.898	1.00 35.51	A
ATOM ATOM	20	0	ASP		4		30.857	8.469	12.170	1.00 25.25	A
ATOM	21	N	HIS		5		30.493	6.277	12.515	1.00 26.22	A
ATOM	22	CA	HIS		5		31.527	6.164	13.544	1.00 26.52	A
MOTA	23	CB	HIS	A	5		30.939	6.339	14.950	1.00 25.34	A
ATOM	24	CG	HIS	A	5		30.240	7.647	15.156	1.00 28.69	A
ATOM	25	CD2	HIS	A	5		30.716	8.870	15.492	1.00 29.15	A
MOTA	26		HIS		5		28.881	7.801	14.979	1.00 28.23	A
MOTA	27		HIS		5		28.550	9.062	15.198	1.00 29.92	A
ATOM	28		HIS		5		29.645	9.732	15.511	1.00 29.84 1.00 25.79	A A
MOTA	29	C	HIS		5 5		32.246 31.630	4.826 3.785	13.465 13.227	1.00 25.79	A
ATOM ATOM	30 31	N O	HIS VAL		6		33.559	4.866	13.659	1.00 24.52	A
ATOM	32	CA	VAL		6		34.385	3.667	13.628	1.00 23.27	A
ATOM	33	CB	VAL		6		35.311	3.657	12.407	1.00 25.22	A
ATOM	34		VAL		6		36.187	2.414	12.440	1.00 24.31	A
MOTA	35	CG2	VAL	A	6		34.489	3.708	11.127	1.00 27.15	A
MOTA	36	С	VAL	A	6		35.256	3.633	14.876	1.00 22.15	A
MOTA	37	0	VAL		6		35.937	4.606	15.185	1.00 21.49	A
MOTA	38	N	ALA		7		35.239	2.513	15.586	1.00 19.90	A
MOTA	39	CA	ALA		7		36.038	2.382	16.799	1.00 19.70 1.00 14.59	A A
ATOM	40	CB C	ALA ALA		7 7		35.132 36.867	2.394 1.111	18.034 16.791	1.00 18.62	A
MOTA MOTA	41 42	0	ALA		7		36.548	0.153	16.088	1.00 20.78	A
ATOM	43	И	SER		8		37.947	1.120	17.560	1.00 16.95	A
ATOM	44	CA	SER		8		38.807	-0.048	17.700	1.00 18.62	A
ATOM	45	СВ	SER		8		40.211	0.215	17.153	1.00 17.69	A
MOTA	46	OG	SER	A	8		40.209	0.271	15,738	1.00 19.81	A
ATOM	47	C	SER	A	8		38.868	-0.310	19.199	1.00 18.76	A
MOTA	48	0	SER		8		39.570	0.376	19.943	1.00 19.35	A
MOTA	49	N	TYR		9		38.070	-1.268	19.645	1.00 19.38 1.00 19.44	A A
MOTA	50	CA	TYR TYR		9		38.038 36.628	-1.608 -1.980	21.048 21.471	1.00 19.44	A
MOTA MOTA	51 52	CB CG	TYR		9 9		35.714	-0.785	21.375	1.00 18.65	A
ATOM	53		TYR		9		36.073	0.435	21.962	1.00 16.57	A
MOTA	54		TYR		9		35.237	1.537	21.897	1.00 17.39	A
MOTA	55		TYR		9		34.493	-0.865	20.716	1.00 17.15	A
MOTA	56	CE2	TYR	A	9		33.641	0.235	20.647	1.00 16.82	A
MOTA	57	CZ	TYR	A	9		34.020	1.431	21.243	1.00 18.07	A
MOTA	58	OH	TYR		9		33.169	2.509	21.210	1.00 19.77	A
MOTA	59	C	TYR		9		38.993	-2.751	21.106	1.00 20.21	A A
ATOM	60	0	TYR		9		38.652	-3.911	21.344	1.00 15.05	A A
MOTA	61 62	N	GLY		10		40.225	-2.357 -3.275	20.831 20.808	1.00 21.69 1.00 22.54	A
MOTA MOTA	62 63	CA C	GLY GLY		10 10		42.276	-3.275	19.655	1.00 21.74	A
MOTA	64	Ö	GLY		10		42.248	-3.863	18.713	1.00 22.02	A
MOTA	65	N	VAL		11		43.083	-2.023	19.674	1.00 18.91	A
ATOM	66	CA	VAL		11		44.119	-1.949	18.651	1.00 17.39	A
MOTA	67	CB	VAL	A	11		44.554	-0.506	18.277		A
MOTA	68		. VAL		11		45.845	-0.558	17.455		A
ATOM	69	CG2	VAL	A	11		43.481	0.165	17.432	1.00 15.25	A

ATOM	70	С	VAL A	11	45.228	-2.644	19.447	1.00 17.05	A
ATOM	71	0	VAL A	11	45.679	-2.145	20.481	1.00 19.34	A
MOTA	72	N	ASN A	12	45.616	-3.828	19.005	1.00 17.39	A
MOTA	73	CA	asn a		46.643	-4.597	19.693	1.00 17.18	A
MOTA	74	CB	asn a		46.113	-5.994	20.052	1.00 15.04	A
MOTA	75	CG	ASN A		44.834	-5.947	20.882	1.00 15.96	A
ATOM	76		ASN A		43.780	-5.490	20.417	1.00 18.20	A
ATOM	77		ASN A		44.921	-6.420	22.114 18.797	1.00 10.46 1.00 18.90	A A
ATOM ATOM	78 79	C 0	ASN A		47.863 47.752	-4.739 -5.162	17.641	1.00 18.80	A
MOTA	80	N	LEU A		49.026	-4.403	19.343	1.00 18.60	A
ATOM	81	CA	LEU A		50.264	-4.478	18.599	1.00 19.90	A
MOTA	82	СВ	LEU A		50.695	-3.064	18.217	1.00 23.26	A
ATOM	83	CG	LEU A	13	52.077	-2.881	17.594	1.00 24.86	A
MOTA	84	CD1	LEU A	. 13	52.085	-3.494	16.201	1.00 26.92	A
ATOM	85	CD2	LEU A	13	52.417	-1.402	17.534	1.00 24.75	A
ATOM	86	C	TEG Y		51.391	-5.165	19.370	1.00 20.37	A
MOTA	87	0	LEU A		51.559	-4.953	20.566	1.00 21.11	A
MOTA	88	N	TYR A		52.145	-6.004	18.673	1.00 21.04	A
ATOM	89	CA	TYR A		53.291 52.909	-6.691 -8.050	19.255 19.844	1.00 24.07 1.00 27.05	A A
ATOM ATOM	90 91	CB	TYR A		54.091	-8.729	20.489	1.00 29.27	A
ATOM	92		TYR A		54.569	-8.304	21.723	1.00 30.07	A
ATOM	93		TYR A		55.709	-8.867	22.285	1.00 31.38	A
ATOM	94		TYR A		54.783	-9.744	19.830	1.00 31.63	A
ATOM	95	CE2	TYR A	14	55.923	-10.314	20.383	1.00 30.29	A
ATOM	96	CZ	TYR A	. 14	56.381	-9.868	21.609	1.00 31.37	A
ATOM	97	OH	TYR A	14	57.515	-10.413	22.160	1.00 34.48	A
MOTA	98	C	TYR A		54.291	-6.900	18.128	1.00 25.30	A
MOTA	99	0	TYR A		53.907	-7.206	16.994	1.00 25.51	A
ATOM	100	N	GLN A		55.571	-6.725	18.429	1.00 24.61 1.00 25.19	A A
ATOM	101	CA	GLN A		56.603 56.932	-6.891 -5.549	17.414 16.754	1.00 23.19	A
ATOM ATOM	102 103	CB	GLN F		57.278	-4.443	17.738	1.00 23.98	A
ATOM	104	CD	GLN A		57.567	-3.116	17.056	1.00 26.32	A
ATOM	105		GLN A		57.575	-2.062	17.702	1.00 28.26	A
ATOM	106	NB2			57.810	-3.159	15.749	1.00 24.64	A
ATOM	107	С	GLN A		57.848	-7.487	18.036	1.00 26.16	A
MOTA	108	0	GLN A	15	58.134	-7.263	19.211	1.00 24.31	A
ATOM	109	N	SER A		58.583	-8.252	17.236	1.00 28.72	A
MOTA	110	CA	SER A		59.801	-8.912	17.698	1.00 30.37	A
ATOM	111	CB	SER A		60.341	-9.830	16.603	1.00 28.35	A N
MOTA	112	OG	SER A		60.569 60.883	-9.100 -7.918	15.407 18.111	1.00 31.43 1.00 32.37	A A
ATOM ATOM	113 114	C O	SER A		61.538	-8.104	19.134	1.00 33.91	A
ATOM	115	N	TYR J		61.073	-6.863	17.325	1.00 32.49	A
ATOM	116	CA	TYR I		62.096		17.664	1.00 34.27	A
MOTA	117	СВ	TYR I		62.172		16.620	1.00 35.41	A
ATOM	118	CG	TYR I	17	63.371	-3.911	16.837	1.00 37.77	A
MOTA	119	CD1	TYR I	17	64.646	-4.347	16.470	1.00 39.38	A
MOTA	120	CB1	TYR I		65.769		16.715	1.00 40.15	A
MOTA	121		TYR		63.247		17.456	1.00 36.31	A
MOTA	122	CE2			64.360		17.707	1.00 39.40 1.00 41.42	A A
ATOM	123	CZ	TYR		65.621 66.732		17.335 17.580	1.00 43.02	A
MOTA MOTA	124 125	C	TYR I		61.821		19.027	1.00 34.43	A
ATOM	126	Ö	TYR		60.765		19.248	1.00 35.58	A
ATOM	127	N	GLY		62.783		19.935	1.00 34.98	A
ATOM	128	CA	GLY :		62.609		21.270	1.00 35.78	A
ATOM	129	C	GLY :		62.730	-5.968	22.292	1.00 36.87	A
MOTA	130	0	GLY :	A 18	63.761	-6.082	22.952	1.00 38.48	A
ATOM	131	N	PRO .		61.692		22.459	1.00 37.06	A
MOTA	132	CD	PRO .		61.745		23.368	1.00 35.58	A
MOTA	133	CA	PRO .		60.409		21.747	1.00 34.79	A
MOTA	134	CB	PRO		59.853		21.981	1.00 35.91 1.00 36.88	A A
MOTA	135	CG	PRO		60.300 59.531		23.394 22.379	1.00 36.88	A A
MOTA	136	C	PRO PRO		59.531 59.844		23.456	1.00 33.71	A
ATOM ATOM	137 138	O N	SER		58.435		21.722	1.00 31.83	A
ATOM	139	CA	SER		57.548		22.290	1.00 30.25	A
MOTA	140	CB	SER		58.060		21.965	1.00 29.00	A
ATOM	141	OG	SER		58.072		20.567	1.00 32.27	A
ATOM	142	C	SER		56.108		21.820	1.00 27.93	A
MOTA	143	0	SER		55.829	-5.129	20.805	1.00 28.23	A

			AT 37			EE 101	-3.911	22.576	1.00 25.87	A
ATOM	144	N	GLY		21	55.191 52.707		.22.222	1.00 23.78	A
ATOM	145	CA	GLY		21	53.797	-2.732		1.00 23.76	A
ATOM	146	C	GLY		21	53.076		22.598	1.00 24.81	
MOTA	147	0	GTA		21	53.638	-1.840	23.247		A
MOTA	148	N	GLN		22	51.821	-2.641	22.187	1.00 20.60	A
MOTA	149	CA	GLN		22	51.033	-1.470	22.495	1.00 19.67	A
MOTA	150	CB	GTN		22	51.239	-0.400	21.415	1.00 19.28	A
ATOM	151	CG	GLN	A	22	50.584	0.943	21.736	1.00 18.12	A
ATOM	152	CD	GLN	A	22	50.732	1.971	20.613	1.00 18.84	A
ATOM	153	OE1	GLN	A	22	51.694	2.749	20.576	1.00 19.77	A
ATOM	154	NE2	GLN	A	22	49.777	1.968	19.688	1.00 16.83	A
ATOM	155	C	GLN	A	22	49.573	-1.873	22.566	1.00 18.66	A
ATOM	156	0	GLN	A	22	49.128	-2.747	21.826	1.00 18.45	A
ATOM	157	N	TYR		23	48.842	-1.257	23.484	1.00 17.25	A
MOTA	158	CA	TYR		23	47.423	-1.529	23.615	1.00 16.53	A
ATOM	159	CB	TYR		23	47.127	-2.497	24.752	1.00 14.51	A
MOTA	160	CG	TYR		23	45.674	-2.904	24.760	1.00 12.67	A
MOTA	161		TYR		23	45.251	-4.070	24.121	1.00 13.38	A
	162		TYR		23	43.904	-4.415	24.070	1.00 13.23	A
ATOM		CD2			23	44.713	-2.093	25.346	1.00 11.07	A
ATOM	163		TYR		23	43.365	-2.425	25.299	1.00 12.99	A
MOTA	164					42.964	-3.583	24.664	1.00 13.72	A
MOTA	165	CZ	TYR		23		-3.907	24.611	1.00 17.15	A
MOTA	166	OH	TYR		23	41.624			1.00 16.88	A
MOTA	167	C	TYR		23	46.694	-0.220	23.860		A
MOTA	168	0	TYR		23	46.975	0.491	24.824	1.00 16.57	
ATOM	169	N	THR		24	45.757	0.085	22.969	1.00 16.16	A
ATOM	170	CA	THR		24	44.975	1.311	23.038	1.00 16.43	A
MOTA	171	CB	THR	A	24	45.594	2.405	22.136	1.00 18.41	A
MOTA	172	0G1	THR	A	24	45.581	1.954	20.771	1.00 17.20	A
ATOM	173	CG2	THR	A	24	47.029	2.692	22.537	1.00 18.64	A
ATOM	174	C	THR	A	24	43.570	1.058	22.499	1.00 15.15	A
MOTA	175	0	THR	Α	24	43.314	0.037	21.879	1.00 15.70	A
MOTA	176	N	HIS	A	25	42.667	1.993	22.754	1.00 15.66	A
ATOM	177	CA	HIS	A	25	41.320	1.924	22.210	1.00 15.79	A
MOTA	178	CB	HIS		25	40.243	1.834	23.297	1.00 13.55	A
ATOM	179	CG	HIS		25	39.956	0.430	23.734	1.00 15.91	A
ATOM	180		HIS		25	40.688	-0.704	23.624	1.00 13.86	A
ATOM	181		HIS		25	38.790	0.071	24.374	1.00 15.91	A
	182		HIS		25	38.815	-1.222	24.639	1.00 14.38	A
ATOM			HIS		25	39.956	-1.715	24.193	1.00 16.99	A
ATOM	183		HIS		25	41.176	3.212	21.437	1.00 14.18	A
ATOM	184	C				41.677	4.241	21.865	1.00 13.52	A
ATOM	185	0	HIS		25		3.150	20.292	1.00 14.81	A
ATOM	186	N		JA	26	40.510		19.462	1.00 16.96	A
ATOM	187	CA		JA	26	40.333	4.329		1.00 16.34	A
MOTA	188	CB		JA	26	41.132	4.188	18.164	1.00 18.80	A
MOTA	189	CG	-	JA	26	42.644	4.158	18.311		A
MOTA	190	œ		JА	26	43.345	4.036	16.958	1.00 22.68	
MOTA	191		LGL		26	42.744	4.456	15.946	1.00 26.77	A
ATOM	192	OE:	2 GL	JA	26	44.490	3.539	16.901	1.00 20.46	A
MOTA	193	C	GLI	JΑ	26	38.875	4.543	19.101	1.00 17.22	A
MOTA	194	0	GL	JA	26	38.104	3.597	18.996	1.00 18.66	A
MOTA	195	N	PH	EΑ	27	38.503	5.802	18.917	1.00 18.91	A
ATOM	196	CA	PH	ΕA	27	37.150	6.135		1.00 19.32	A
MOTA	197	CB	PH	ΕA	. 27	36.290	6.546	19.698	1.00 20.19	A
MOTA	198	CG	PH	ΕA	. 27	34.834	6.653	19.357	1.00 23.33	A
MOTA	199	CD	1 PH	E A	27	34.024	5.524	19.360	1.00 22.07	A
MOTA	200	æ	2 PH	E A	27	34.289	7.868	18.971	1.00 23.24	A
MOTA	201		1 PH			32.692	5.606	18.980	1.00 26.16	A
ATOM	202		2 PH			32.954	7.962	18.587	1.00 25.99	A
ATOM	203			E A		32.155	6.828		1.00 25.46	A
ATOM	204			E A		37.260	7.291		1.00 19.10	A
ATOM	205			ΕA		37.733	8.375		1.00 19.83	A
				PA		36.831				A
MOTA	206			PA		36.901				A
MOTA	207			PA		35.910				A
MOTA	208					34.472				A
ATOM	209		1 AS	PA						A
MOTA	210					34.266				A
ATOM	211		2 AS			33.552				A
MOTA	212			P		38.297				A
MOTA	213			P I		38.467				A
MOTA	214			Y		39.292				A
MOTA	215			Y Z		40.658				
MOTA	216			ΥZ		41.437				A
MOTA	217	7 0	ĢI	X I	A 29	42.621	9.010	15.814	1.00 19.26	A

ATOM	218	N	ASP		30	40.797	8.922	17.098	1.00 16.92	A
MOTA	219	CA	ASP		30	41.511	9.438	18.254	1.00 16.83	A
MOTA	220	CB CG	ASP ASP		30 30	40.816 40.988	10.678 11.864	18.796 17.888	1.00 18.99 1.00 21.09	A A
ATOM ATOM	221 222		ASP		30	42.145	12.177	17.538	1.00 22.94	A
ATOM	223		ASP		30	39.971	12.478	17.525	1.00 21.68	A
MOTA	224	C	ASP	A	30	41.656	8.392	19.345	1.00 17.25	A
MOTA	225	0	ASP		30	40.777	7.553	19.543	1.00 15.40	A
ATOM	226	N	GLU		31	42.784	8.453	20.041	1.00 16.77 1.00 18.43	A A
ATOM	227	CA	GLU		31 31	43.111 44.620	7.514 7.607	21.107 21.392	1.00 20.90	A
ATOM ATOM	228 229	CB CG	GTA		31	45.147	6.853	22.608	1.00 24.68	A
ATOM	230	CD	GLU		31	46.678	6.924	22.702	1.00 27.25	A
ATOM	231		GLU	A	31	47.258	7.931	22.239	1.00 26.93	A
MOTA	232		GLU		31	47.302	5.985	23.242	1.00 27.21	A
ATOM	233	C	GLU		31	42.296 42.361	7.777 8.863	22.375 22.952	1.00 17.51 1.00 17.13	A A
ATOM ATOM	234 235	N O	GLU		31 32	41.525	6.784	22.807	1.00 15.52	A
MOTA	236	CA	GLN		32	40.726	6.942	24.020	1.00 16.47	A
MOTA	237	CB	GLN		32	39.542	5.980	24.009	1.00 15.91	A
ATOM	238	CG	GLN		32	38.439	6.399	23.065	1.00 15.97	A
MOTA	239	CD	GLN		32	37.292	5.419	23.071	1.00 20.20 1.00 18.09	A A
ATOM	240		GLN		32 32	37.478 36.091	4.228 5.912	22.808 23.374	1.00 20.57	Ā
MOTA MOTA	241 242	NE2 C	GLIN		32	41.584	6.701	25.255	1.00 16.61	A
ATOM	243	ŏ	GLN		32	41.448	7.387	26.272	1.00 15.51	A
MOTA	244	N	PHE		33	42.470	5.720	25.151	1.00 15.59	A
MOTA	245	CA	PHE		33	43.370	5.389	26.239	1.00 16.34	A
MOTA	246	CB	PHE		33	42.583	4.854 3.502	27.443 27.222	1.00 17.21 1.00 16.68	A A
ATOM ATOM	247 248	CG	PHE PHE		33 33	41.951 42.686	2.333	27.406	1.00 15.57	A
ATOM	249		PHE		33	40.598	3.397	26.903	1.00 18.54	A
ATOM	250		PHE		33	42.083	1.076	27.288	1.00 16.34	A
MOTA	251		PHE		33	39.983	2.147	26.782	1.00 17.35	A
MOTA	252	CZ	PHE		33	40.729	0.983	26.978 25.776	1.00 16.56 1.00 16.66	A A
ATOM	253	0	PHE		33 33	44.363 44.209	4.343	24.712	1.00 16.85	A
ATOM ATOM	254 255	N	TYF		34	45.398	4.139	26.572	1.00 16.03	A
ATOM	256	CA	TYF		34	46.377	3.125	26.264	1.00 16.93	A
ATOM	257	CB	TY	A S	34	47.636	3.730	25.621	1.00 16.33	A
ATOM	258	CG		A S	34	48.528	4.541	26.523	1.00 17.31 1.00 17.48	A A
MOTA	259		L TYI		34 34	49.519 50.367	3.930 4.683	27.291 28.097	1.00 17.40	A
MOTA MOTA	260 261		TY		34	48.404	5.928	26.586	1.00 17.68	A
MOTA	262		TY		34	49.244	6.690	27.388	1.00 19.73	A
MOTA	263	CZ	TYI	R A	34	50.224	6.060	28.141	1.00 20.10	A
MOTA	264	OH		R A	34	51.044	6.815	28.941	1.00 23.02 1.00 17.88	A A
MOTA	265	C		R A R A	34 34	46.692 46.429	2.473 3.042	27.588 28.646	1.00 17.00	A
ATOM ATOM	266 267	Ŋ		LA	35	47.213	1.261	27.535	1.00 17.31	A
MOTA	268	CA		ЬA		47.571	0.570	28.749	1.00 18.89	A
MOTA	269	CB	VA	LΑ	35	46.950	-0.848	28.804	1.00 19.12	A
MOTA	270		1 VA			47.589	-1.660	29.912	1.00 17.56 1.00 19.75	A A
MOTA	271	-	2 VA	LА LА		45.454 49.084	-0.742 0.478		1.00 18.84	A
MOTA MOTA	272 273			LA		49.701	-0.050			A
MOTA	274			PA		49.676	1.039		1.00 22.55	A
MOTA	275		AS	P A	. 36	51.121				A
ATOM	276			P A		51.542				A A
MOTA	277		AS 1 AS	PA		53.033 53.796				A
MOTA MOTA	278 279		1 AS			53.441				A
MOTA	280			P P		51.393			1.00 26.39	A
MOTA	281		AS	P A	36	51.016	-0.976			A
ATOM	282			U		52.024				A
MOTA	283			ינדי <i>ד</i>		52.305				A A
MOTA MOTA	284 285			נט: נט:		52.754 51.704				A
MOTA	286		1 LE			52.265			1.00 21.32	A
ATOM	287		2 L			50.455	-3.876	27.557		A
MOTA	288	3 C		EU 2		53.348				A
MOTA	289			3U 1		53.222				A A
MOTA	290 291			TA 1		54.362 55.403				Ã
MOTA	43.		,	•		22			_	

MOTA	292	С	GLY	A	38	54.956	-1.863	33.162	1.00 37.63	A
MOTA	293		GLY		38	55.369	-2.549	34.098	1.00 38.42	A
MOTA			ARG		39	54.101	-0.861	33.334	1.00 38.93 1.00 40.81	A A
ATOM	295		ARG ARG		39 39	53.625 53.645	-0.499 1.029	34.660 34.803	1.00 42.41	A
MOTA MOTA	296 297	CB CG	ARG		39	54.968	1.627	34.339	1.00 44.76	A
ATOM	298	CD	ARG		39	55.113	3.118	34.619	1.00 47.83	A
ATOM	299	NE	arg	A	39	56.318	3.644	33.976	1.00 50.52	A
ATOM	300	CZ	ARG		39	56.902	4.799	34.281	1.00 53.40	A
MOTA	301	NHl			39	56.399	5.575	35.235 33.633	1.00 54.01 1.00 54.18	A A
MOTA	302	NH2 C	ARG ARG		39 39	57.998 52.229	5.179 -1.057	34.936	1.00 41.12	A
ATOM ATOM	303 304	0	ARG		39	51.664	-0.847	36.014	1.00 39.71	A
ATOM	305	N	LYS		40	51.687	-1.779	33.955	1.00 40.65	A
ATOM	306	CA	LYS	A	40	50.365	-2.380	34.070	1.00 39.55	A
MOTA	307	СВ	LYS		40	50.415	-3.554	35.053	1.00 42.42 1.00 46.46	A A
ATOM	308	CG	LYS		40	49.196 49.266	-4.467 -5.563	34.996 36.054	1.00 50.42	A
ATOM	309 310	CD CE	LYS		40 40	48.077	-6.513	35.947	1.00 51.25	A
MOTA MOTA	311	NZ	LYS		40	46.781	-5.779	35.970	1.00 52.15	A
ATOM	312	C	LYS		40	49.338	-1.348	34.540	1.00 37.45	A
ATOM	313	0	LYS		40	48.647	-1.560	35.533	1.00 35.78	A
MOTA	314	N	GLU		41	49.245	-0.237 0.847	33.812 34.142	1.00 35.81 1.00 33.83	A A
ATOM	315	CA	GLU		41 41	48.317 49.077	2.079	34.655	1.00 36.46	A
MOTA MOTA	316 317	CB CG	GLU		41	49.660	1.997	36.049	1.00 41.33	A
ATOM	318	CD	GLU		41	50.500	3.224	36.374	1.00 44.23	A
ATOM	319	OB1	GLU	Α	41	50.067	4.343	36.022	1.00 46.67	A
MOTA	320	OE2			41	51.585	3.076	36.981 32.937	1.00 45.55 1.00 30.89	A A
MOTA	321	C	GLU		41 41	47.492 47.995	1.301 1.373	31.816	1.00 27.89	A
MOTA MOTA	322 323	O N	GLU		42	46.227	1.623	33.182	1.00 28.11	A
ATOM	324	CA	THE		42	45.354	2.127	32.135	1.00 26.58	A
MOTA	325	CB	THE		42	43.882	1,773	32.406	1.00 27.67	A
MOTA	326		THE		42	43.716	0.349	32.394	1.00 25.55 1.00 25.33	A A
MOTA	327		THE		42	42.979 45.506	2.419 3.642	31.357 32.212	1.00 26.90	A
MOTA	328 329	C O	THE		42 42	45.305	4.232	33.269	1.00 25.79	A
ATOM ATOM	330	N	VAI		43	45.881	4.273	31.108	1.00 25.87	A
ATOM	331	CA	VAI	A	43	46.045	5.720	31.106	1.00 24.36	A
MOTA	332	СВ		A	43	47.474	6.119	30.670	1.00 24.45 1.00 24.38	A A
MOTA	333	CG1			43	47.698 48.504	7.606 5.289	30.906 31.433	1.00 22.82	A
MOTA MOTA	334 335	C	IAV :	A	43 43	45.039	6.331	30.141	1.00 24.94	A
ATOM	336	ō		LA	43	45.143	6.133	28.930	1.00 24.72	A
ATOM	337	N		PA	44	44.063	7.065	30.672	1.00 24.50	A
ATOM	338	CA		PA	44	43.050	7.681	29.824	1.00 25.64 1.00 25.03	A A
ATOM	339	СВ		A q	44	41.804	8.033 6.859	30.642 31.370	1.00 25.05	A
MOTA	340 341	CG	TR	PA	44 44	40.281	5.906	30.858	1.00 25.77	A
ATOM ATOM	342		2 TR		44	40.067	4.946	31.870	1.00 26.64	A
ATOM	343		TR		44	39.599	5.766	29.641	1.00 24.94	A
MOTA	344		l TR		44	41.529	6.450	32.634	1.00 26.43 1.00 26.28	A A
MOTA	345		1 TR 2 TR			40.840 39.197		32.942 31.704	1.00 25.25	A
MOTA	346 347		2 TR 3 TR			38.734			1.00 22.40	A
MOTA MOTA	348		2 TR			38.542			1.00 24.18	A
MOTA	349	C	TR	P A	44	43.578			1.00 26.30	A
ATOM	350	0		PA		44.321				A A
MOTA	351	N		s a s a		43.193 43.635				Ä
MOTA	352 353			SA		44.069				A
MOTA MOTA	354			SA		45.547			1.00 30.66	A
MOTA	355		CX	S A	45	42.574				A
MOTA	356			SA		42.836				A A
MOTA	357			A UE		41.375				Ā
MOTA	358 359			SU A		39.137				A
MOTA MOTA	360			U A		38.810		25.263	1.00 32.47	A
ATOM	361	. CI	1 Li	T DE	46	37.492				A
MOTA	362		2 Ы			38.71				A A
MOTA	363			3U #		39.734 39.19				A
MOTA MOTA	364 369			EU 1 RO 1		39.19				A
WT OU	50.									

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ATOM	366	CD	PRO		47	40.488	14.442	28.986	1.00 32.23	A
ATOM	367	CA	PRO		47	39.437	13.392	30.901	1.00 32.18	A
ATOM	368	CB	PRO	A	47	39.487	14.908	31.063	1.00 32.11	A
MOTA	369	CG	PRO	A	47	40.690	15.270	30.236	1.00 31.60	A
MOTA	370	C	PRO	A	47	38.066	12.800	31.245	1.00 30.96	A
ATOM	371	0	PRO	A	47	37.927	12.103	32.243	1.00 30.17	A
ATOM	372	N	VAL	A	48	37.064	13.068	30.418	1.00 30.75	A
ATOM	373	CA	VAL	A	48	35.715	12.563	30.663	1.00 32.56	A
ATOM	374	CB	VAL	A	48	34.748	13.040	29.560	1.00 34.04	A
ATOM	375	CG1	VAL	A	48	33.320	12.683	29.932	1.00 34.16	A
MOTA	376	CG2	VAL	A	48	34.881	14.556	29.368	1.00 38.02	A
ATOM	377	С	VAL	A	48	35.633	11.033	30.765	1.00 33.13	A
MOTA	378	0	VAL	A	48	34.698	10.485	31.355	1.00 33.55	A
ATOM	379	N	LEU	A	49	36.615	10.350	30.192	1.00 33.30	A
MOTA	380	CA	LEU	A	49	36.661	8.892	30.208	1.00 32.44	A
MOTA	381	CB	LEU	A	49	37.498	8.391	29.023	1.00 30.62	A
MOTA	382	CG	LEU	A	49	36.792	8.027	27.702	1.00 31.64	A
ATOM -	383	CD1	LEU	A	49	35.578	8.888	27.464	1.00 29.12	A
MOTA	384	CD2	LEU	A	49	37.783	8.157	26.551	1.00 31.05	A
ATOM	385	C	LEU	A	49	37.226	8.343	31.519	1.00 33.77	A
ATOM	386	0	LEU		49	37.138	7.142	31.787	1.00 34.14	A
ATOM	387	N	ARG		50	37.794	9.221	32.339	1.00 34.56	A
ATOM	388	CA	ARG		50	38.367	8.810	33.618	1.00 35.58	A
ATOM	389	CB	ARG		50	38.987	10.009	34.345	1.00 37.99	A
MOTA	390	CG	ARG		50	40.137	10.720	33.636	1.00 40.65	A
ATOM	391	CD	ARG		50	40.657	11.846	34.529	1.00 43.05	A
ATOM	392	NE	ARG		50	41.603	12.748	33.872	1.00 44.85	A
MOTA	393	CZ	ARG		50	42.815	12.403	33.444	1.00 46.08	A
MOTA	394	NH1			50	43.254	11.159	33.592	1.00 46.76	A
ATOM	395	NH2			50	43.599	13.314	32.880	1.00 46.08	A
ATOM	396	C	ARG		50	37.334	8.168	34.547	1.00 35.55	A
ATOM	397	ō	ARG		50	37.693	7.475	35.495	1.00 35.21	A
ATOM	398	N	GLN		51	36.054	8.412	34.284	1.00 36.77	A
ATOM	399	CA	GLN		51	34.987	7.859	35.116	1.00 37.34	A
	400	CB	GLN		51	33.658	8.558	34.821	1.00 39.02	A
ATOM ATOM	401	CG	GLN		51	33.123	8.306	33.418	1.00 41.24	A
		CD	GLN		51	31.765	8.947	33.189	1.00 43.49	A
ATOM	402		GLN		51	30.781	8.597	33.843	1.00 43.80	A
ATOM	403	NE2			51	31.706	9.895	32.260	1.00 44.01	A
ATOM	404		GLN		51	34.821	6.362	34.896	1.00 36.85	A
ATOM	405	C				34.250	5.665	35.734	1.00 37.06	A
ATOM	406	0	GLN		51		5.871	33.764	1.00 37.00	A
MOTA	407	N	PHE		52 53	35.316	4.454	33.446	1.00 32.82	A
MOTA	408	CA	PHE		52	35.218		31.931	1.00 31.28	A
MOTA	409	CB	PHE		52	35.143	4.258	31.301	1.00 31.26	A
MOTA	410	CG	PHE		52	33.902	4.838	31.821	1.00 27.82	A
MOTA	411		PHE		52	32.640	4.549 5.652	30.177	1.00 27.71	A
MOTA	412		PHE		52	33.992		31.234	1.00 27.71	A
MOTA	413		PHE		52	31.490	5.060 6.171		1.00 28.10	A
MOTA	414		PHE		52	32.847		29.580 30.111	1.00 28.21	A
ATOM	415	CZ	PHE		52	31.592	5.873	34.004	1.00 32.57	A
ATOM	416	C	PHE		52	36.405	3.675	34.494	1.00 32.37	A
ATOM	417	0	PHE		52	37.370	4.256 2.353		1.00 32.22	Ā
MOTA	418	N	ARG		53	36.327		33.927		A
MOTA	419	CA	ARG		53	37.397	1.498 0.862	34.419 35.760	1.00 32.77 1.00 36.56	A
MOTA	420	CB	ARG		53	37.005			1.00 42.83	
ATOM	421	CG	ARG		53	36.741	1.867	36.881 38.214	1.00 42.83	A A
ATOM	422	CD	ARG		53	36.523	1.168 2.111		1.00 53.82	Ä
MOTA	423	NE	ARG		53	36.308		39.312 40.589	1.00 54.70	Ä
MOTA	424	CZ	ARG		53	36.195	1.758		1.00 54.70	A
MOTA	425		ARG		53	36.277	0.478	40.937		
MOTA	426		ARG		53	36.004	2.683	41.520	1.00 55.64	A
MOTA	427	C	ARG		53	37.706	0.404	33.405	1.00 29.88	A
MOTA	428	0	ARC		53	36.806	-0.117	32.743	1.00 28.71	A
MOTA	429	N	PHE		54	38.986	0.066	33.293	1.00 26.44	A
MOTA	430	CA		A	54	39.440	-0.960		1.00 22.47	A
MOTA	431	CB		A	54	39.905	-0.325		1.00 21.88	A
MOTA	432	CG		3 A	54	40.181			1.00 20.69	A
MOTA	433		L PHI		54	39.150	-1.801		1.00 19.52	A
MOTA	434		2 PHI		54	41.471	-1.782		1.00 18.68	A
MOTA	435		L PHI		54	39.399			1.00 22.81	A
MOTA	436		2 PHI		54	41.733			1.00 20.58	A
MOTA	437	CZ		E A	54	40.697			1.00 20.86	A
MOTA	438	C		BA	54	40.597				A.
MOTA	439	0	PH	E A	54	41.631	-1.122	33.351	1.00 23.53	A

MOTA	440	N	ASP	Δ.	55	40.408	-3.011	33.198	1.00 22.82	A
ATOM	441	CA	ASP		55	41.411	-3.874	33.805	1.00 24.70	A
ATOM	442	CB	ASP		55	40.785	-5.246	34.083	1.00 23.26	A
ATOM	443	CG	ASP		55	41.729	-6.190	34.789	1.00 26.24	A
ATOM	444		ASP		55	42.924	-5.853	34.933	1.00 28.75	A
ATOM	445		ASP		55	41.274	-7.279	35.192	1.00 26.38	A
ATOM	446	C	ASP		55	42.613	-4.011	32.861	1.00 24.24	A
ATOM	447	0	ASP		55	42.510	-4.629	31.802	1.00 23.91	A
ATOM	448	И	PRO		56	43.770	-3.437	33.238	1.00 23.69	A
ATOM	449	CD .	PRO		56	44.084	-2.761	34.509	1.00 23.79	A
ATOM	450	CA	PRO		56	44.961	-3.522	32.387	1,00 23.45	A
ATOM	451	CB	PRO		56	46.002	-2.707	33.162	1.00 23.35	A
ATOM	452	CG	PRO		56	45.592	-2.897	34.580	1.00 23.31	A
ATOM	453	C	PRO		56	45.413	-4.952	32.114	1.00 23.66	A
ATOM	454	ō	PRO		56	46.099	-5.220	31,125	1.00 23.15	A
MOTA	455	N	GLN		57	45.025	-5.871	32.991	1.00 21.84	A
ATOM	456	CA	GLN		57	45.397	-7.261	32.818	1.00 22.47	A
ATOM	457	СВ	GITN		57	44.834	-8.108	33.965	1.00 23.11	A
ATOM	458	CG	GLN		57	45.226	-9.568	33.873	1.00 20.82	A
MOTA	459	CD	GLN		57	46.722	-9.745	33.733	1.00 22.23	A
ATOM	460		GLN		57	47.497	-9.227	34.539	1.00 21.88	A
MOTA	461		GLN		57	47.138		32.707	1.00 23.15	A
ATOM	462	C	GLN		57	44.882	-7.792	31.482	1.00 22.21	A
ATOM	463	Ö	GLN		57	45.452	-8.723	30.913	1.00 23.00	A
ATOM	464	И	PHE		58	43.801	-7.203	30.980	1.00 22.42	A
ATOM	465	CA	PHE		58	43.254	-7.640	29.704	1.00 21.07	A
ATOM	466	СВ	PHE		58	42.004	-6.857	29.338	1.00 20.45	A
ATOM	467	CG	PHE		58	41.411	-7.287	28.031	1.00 21.03	A
ATOM	468		PHE		58	40.472	-8.312	27.988	1.00 18.42	A
ATOM	469		PHE		58	41.864	-6.736	26.835	1.00 18.79	A
ATOM	470		PHE		58	39.992	-8.792	26.765	1.00 21.25	A
ATOM	471		PHE		58	41.393	-7.207	25.610	1.00 20.28	A
MOTA	472	CZ	PHE		58	40.457	-8.238	25.578	1.00 21.18	A
MOTA	473	C	PHE		58	44.278	-7.401	28.612	1.00 21.79	A
MOTA	474	ō	PHE		58	44.529	-8.260	27.763	1.00 21.84	A
MOTA	475	N	ALA		59	44.849	-6.202	28.637	1.00 21.80	A
ATOM	476	CA	ALA		59	45.840	-5.801	27.657	1.00 21.67	A
MOTA	477	СВ	ALA		59	46.254	-4.346	27.892	1.00 21.11	A
ATOM	478	C	ALA		59	47.053	-6.711	27.732	1.00 22.06	A
ATOM	479	0	ALA		59	47.518	-7.213	26.706	1.00 22.53	A
ATOM	480	N	LEU		60	47.561	-6.925	28.945	1.00 19.83	A
ATOM	481	CA	LEU		60	48.729	-7.777	29.116	1.00 20.88	A
ATOM	482	CB	LEU		60	49.163	-7.815	30.585	1.00 20.57	A
ATOM	483	CG	LEC		60	50.060	-6.657	31.053	1.00 24.17	A
ATOM	484		LEC		60	49.239	-5.392	31.205	1,00 24.16	A
ATOM	485		LEC	-	60	50.717	-7.012	32.382	1.00 24.31	A
MOTA	486	c	LEC		60	48.496	-9.193	28.598	1.00 20.44	A
MOTA	487	ō	LEC		60	49.367	-9.770	27.955	1.00 21.97	A
ATOM	488	N	THE		61	47.319	-9.749	28.871	1.00 20.69	A
ATOM	489	CA		A	61	46.997	-11.101	28.418	1.00 19.49	A
ATOM	490	СВ		A	61	45.697	-11.629	29.084	1.00 18.59	A
ATOM	491	OG:			61	45.919	-11.830	30.489	1.00 21.12	A
ATOM	492	CG	2 THE	A S	61	45.274	-12.942	28.453	1.00 17.61	A
ATOM	493	C	THE	A S	61	46.834	-11.140	26.903	1.00 19.22	A
ATOM	494	0	TH	R A	61	47.325	-12.059	26.242	1.00 21.19	A
MOTA	495	N	ASI	A D	62	46.152	-10.142	26.351	1.00 18.05	A
ATOM	496	CA	ASI	A	62	45.934	-10.092	24.910	1.00 19.26	A
MOTA	497	СВ	AS	A R	62	45.020	-8.910	24.552	1.00 20.51	A
MOTA	498	CG	AS	A R	62	43.835	-9.324	23.680	1.00 22.06	A
MOTA	499	OD	1 AS	A R	62	43.406	-10.482	23.693	1.00 21.71	A
MOTA	500	ND	2 AS	A R	62	43.294	-8.371	22.930		A
MOTA	501	C	AS:	A N	62	47.270	-9.975			A
MOTA	502	0	AS	A N	62	47.517	-10.681			A
MOTA	503	N	IL	B A	63	48.146				A
MOTA	504			B A		49.448				A
ATOM	505			E A		50.229				A
MOTA	506		2 IL			51.601				A
MOTA	507		1 IL			49.425				A
MOTA	508		1 IL			49.037				A
ATOM	509			e a			-10.212			A
MOTA	510			E A			-10.538			A
MOTA	511			A A			-10.949			A
MOTA	512			A A			-12.222			A
ATOM	513	CE	AL	A A	64	50.373	-12.816	26.785	1.00 22.29	A

ATOM	514	C	ALA 2	A.	64	50.252 -13.158 24.301 1.00 23.03	A
MOTA	515	0	ALA 2	A.	64	51.032 -13.939 23.766 1.00 25.08	A
MOTA	516	N	VAL 2		65	48.976 -13.072 23.948 1.00 23.28	A
MOTA	517	CA	VAL		65	48.437 -13.905 22.888 1.00 22.97	A
ATOM	518	CB	VAL 2		65	46.887 -13.840 22.859 1.00 24.28 46.338 -14.722 21.729 1.00 22.40	A A
ATOM ATOM	519 520		VAL X		65 65	46.325 -14.296 24.209 1.00 19.61	A
ATOM	521	C	VAL		65	49.013 -13.471 21.538 1.00 23.88	A
MOTA	522	ō	VAL		65	49.313 -14.314 20.692 1.00 22.01	A
ATOM	523	N	LEU		66	49.179 -12.164 21.332 1.00 24.00	A
ATOM	524	CA	LEU .		66	49.747 -11.692 20.064 1.00 24.66	A
ATOM	525	CB	LEU .	A	66	49.872 -10.171 20.011 1.00 22.13	A
MOTA	526	CG	LEU .	A	66	48.679 -9.228 20.117 1.00 23.81	A
MOTA	527		LEU .		66	49.014 -8.001 19.277 1.00 20.24	A
ATOM	528		LEU .		66	47.407 -9.866 19.627 1.00 20.49	A
ATOM	529	C	LEU .		66	51.143 -12.267 19.906 1.00 23.53 51.548 -12.644 18.813 1.00 22.08	A A
ATOM	530	0	LEU		66 67	51.548 -12.644 18.813 1.00 22.08 51.879 -12.303 21.011 1.00 26.17	A
MOTA MOTA	531 532	N CA	LYS		67	53.237 -12.832 21.019 1.00 28.99	A
ATOM	533	СВ	LYS		67	53.839 -12.698 22.421 1.00 29.27	A
ATOM	534	CG	LYS		67	55.278 -13.174 22.548 1.00 30.64	A
ATOM	535	CD	LYS		67	55.779 -13.001 23.976 1.00 32.41	A
ATOM .	536	CE	LYS	A	67	57.159 -13.609 24.157 1.00 35.25	A
MOTA	537	NZ	LYS	A	67	58.144 -13.036 23.199 1.00 38.78	A
ATOM	538	C	LYS		67	53.200 -14.299 20.598 1.00 29.87	A
MOTA	539	0	LYS		67	53.952 -14.719 19.716 1.00 30.35	A
ATOM	540	N	HIS		68	52.313 -15.066 21.230 1.00 30.48 52.163 -16.483 20.922 1.00 31.95	A A
ATOM	541	CA	HIS		68	52.163 -16.483 20.922 1.00 31.95 51.051 -17.097 21.775 1.00 34.42	A
MOTA MOTA	542 543	CB CG	HIS HIS		68 68	50.827 -18.557 21.520 1.00 38.63	A
ATOM	544		HIS		68 .	49.859 -19.203 20.826 1.00 40.18	A
ATOM	545		HIS		68	51.676 -19.536 21.992 1.00 41.00	A
ATOM	546		HIS		68	51.241 -20.721 21.601 1.00 39.93	A
MOTA	547	NE2	HIS	A	68	50.141 -20.547 20.891 1.00 39.69	A
MOTA	548	C	HIS	A	68	51.828 -16.660 19.448 1.00 31.53	A
MOTA	549	0	HIS		68	52.463 -17.447 18.746 1.00 32.07	A
MOTA	550	N	asn		69	50.826 -15.928 18.977 1.00 29.53	A
MOTA	551	CA	ASN		69	50.427 -16.024 17.583 1.00 29.99	A A
MOTA	552	СВ	ASN		69	49.180 -15.173 17.332 1.00 30.27 47.918 -15.814 17.885 1.00 31.83	A
MOTA	553	CG	ASN ASN		69 69	47.918 -15.814 17.885 1.00 31.83 47.986 -16.728 18.703 1.00 32.19	A
ATOM ATOM	554 555		ASN		69	46.759 -15.328 17.447 1.00 31.41	A
ATOM	556	c	ASN		69	51.552 -15.602 16.638 1.00 30.37	A
ATOM	557	ō	ASN		69	51.722 -16.186 15.571 1.00 29.41	A
ATOM	558	N	LEU		70	52.324 -14.593 17.026 1.00 29.86	A
ATOM	559	CA	LEU	A	70	53.413 -14.131 16.175 1.00 31.35	A
MOTA	560	CB	LEU	A	70	54.039 -12.857 16.751 1.00 28.55	A
MOTA	561	CG	LEU		70	55.190 -12.237 15.950 1.00 28.77	A
MOTA	562		LEU		70	54.745 -11.949 14.519 1.00 28.48	A A
MOTA	563		LEU		70 70	55.651 -10.957 16.627 1.00 27.89 54.479 -15.214 16.009 1.00 31.92	A
ATOM	564 565	C	Tea Tea		70 70	54.994 -15.422 14.914 1.00 31.72	A
MOTA MOTA	566	Ŋ	ASN		71	54.798 -15.905 17.097 1.00 34.09	A
ATOM	567	CA	ASN		71	55.801 -16.968 17.060 1.00 38.27	A
ATOM	568	CB	ASN		71	55.884 -17.651 18.427 1.00 39.70	A
ATOM	569	CG	asn	A	71	56.490 -16.748 19.490 1.00 44.05	A
ATOM	570	OD:	nra j	A	71	56.290 -16.955 20.693 1.00 44.98	A
MOTA	571		2 ASN		71	57.247 -15.746 19.049 1.00 44.44	A
MOTA	572	C	ASN		71	55.484 -18.003 15.983 1.00 38.32 56.358 -18.417 15.224 1.00 37.91	A A
MOTA	573	0	ASN		71	56.358 -18.417 15.224 1.00 37.91 54.221 -18.407 15.919 1.00 39.49	A
ATOM ATOM	574 575	N CA	SER SER		72 72	53.780 -19.390 14.944 1.00 40.10	A
MOTA	576	CB	SER		72	52.341 -19.816 15.256 1.00 41.05	A
ATOM	577	OG	SER		72	51.867 -20.763 14.311 1.00 42.44	A
ATOM	578	C	SER		72	53.860 -18.838 13.523 1.00 40.66	A
ATOM	579		SER		72	54.336 -19.516 12.608 1.00 40.90	A
MOTA	580	N	LEU		73	53.391 -17.608 13.341 1.00 39.86	A
MOTA	581				73	53.408 -16.973 12.030 1.00 39.32	A
ATOM	582		LEU		73	52.676 -15.632 12.082 1.00 38.99	A A
ATOM	583				73 73	51.221 -15.651 11.598 1.00 40.31 50.482 -16.860 12.152 1.00 39.79	A
MOTA	584 585		2 LEU		73 73	50.482 -16.860 12.152 1.00 39.79 50.539 -14.363 12.024 1.00 40.04	A.
MOTA MOTA	586		LEU			54.816 -16.778 11.492 1.00 38.55	A
ATOM	587		LEU			55.028 -16.806 10.280 1.00 36.83	A

MOTA	588	N	ILE	A	74		0 39.70	A
MOTA	589	CA	ILE		74		0 41.87	A A
MOTA	590	CB		A	74		0 41.88 0 41.29	A
ATOM ATOM	591 592	CG2 CG1	ILE		74 74		0 41.53	A
ATOM	593		ILE		74		0 40.94	A
ATOM	594	C	ILE		74	•	0 42.04	A
ATOM	595	0	ILE	A	74		0 41.12	A
ATOM	596	N	LYS		75		0 43.51	A
ATOM	597	CA	LYS		75		0 46.61 0 47.84	A A
ATOM	598	CB CG	LYS		75 75	• • • • • • • • • • • • • • • • • • • •	0 50.82	A
ATOM ATOM	599 600	CD	LYS		75		0 53.97	A
MOTA	601	CE	LYS		75	58.005 -21.646 -16.269 1.0	0 55.95	· A
MOTA	602	NZ	LYS		75		0 56.31	A
MOTA	603	C	LYS		75	201201	0 47.99	A A
MOTA	604	0	LYS		75		0 48.11 0 49.31	A
MOTA	605	N CA	ARG		76 76	• • • • • • • • • • • • • • • • • • • •	0 50.89	A
ATOM ATOM	606 607	СВ	ARG		76		0 53.08	A
ATOM	608	CG	ARG		76		0 56.83	A
ATOM	609	CD	ARG	A	76		0 58.85	A
ATOM	610	NE	ARG		76		0 60.24	A A
MOTA	611	CZ	ARG		76		0 61.29 0 60.08	A
ATOM	612	NH1 NH2	ARG ARG		76 76		0 61.97	A
ATOM ATOM	613 614	C	ARG		76		0 50.93	A
ATOM	615	ŏ	ARG		76		0 51.19	A
ATOM	616	N	SER	A	77		0 50.61	A
MOTA	617	CA	SER		77		00 50.08	A A
ATOM	618	CB	SER		77		00 50.05 00 49.23	A
MOTA	619	OG C	SER SER		77 77	30.220 20	0 49.56	A
ATOM ATOM	620 621	0	SER		77		0 49.40	A
MOTA	622	N	ASN		78		00 49.24	A
ATOM	623	CA	asn		78	001200	00 49.14	A
MOTA	624	CB	ASN		78		00 48.86	A
MOTA	625	CG	ASN		78		00 48.09 00 46.05	A A
MOTA	626		. ASN . ASN		78 78		00 47.78	A
MOTA MOTA	627 628	C	ASN		78	******	00 49.08	A
ATOM	629	ō	ASN		78		00 48.39	A
MOTA	630	N	SER	A S	79		00 48.58	A
MOTA	631	CA	SER		79	00,220	00 48.38	A A
MOTA	632	CB	SEF		79 70		00 48.53 00 50.05	A
MOTA MOTA	633 634	OG C	SEF		79 79		00 47.13	A
MOTA	635	Ö	SEF		79		00 47.66	A
MOTA	636	N	THE		80		00 45.82	A
MOTA	637	CA	THE	R A	80		00 45.51	A
MOTA	638	CB	THE		80		00 47.03	A A
ATOM	639	OG:			80		00 47.95 00 47.59	Ā
MOTA MOTA	640 641		THE	R A			00 44.25	A
MOTA	642			RA		57.835 -11.976 7.556 1.	00 43.69	A
ATOM	643			A A			00 41.47	A
ATOM	644	CA		A A			00 38.59	A
MOTA	645			A A		• • • • • • • • • • • • • • • • • • • •	00 38.61 00 36.89	A A
MOTA	646 647			A A A A			00 35.83	A
MOTA MOTA	648			A A			00 34.86	A
MOTA	649			A A		58.300 -6.690 7.698 1.	00 33.41	A
MOTA	650	СВ	AL	A A	82	## The state of th	00 34.17	A
MOTA	651			A A			.00 32.28 .00 28.62	A A
MOTA	652			A A			00 28.62	A
MOTA MOTA	653 654			RA RA		55.15.	.00 32.87	A
ATOM	659			RA			00 34.31	A
ATOM	656		1 TH			58.347 -5.562 3.058 1.	.00 36.90	A
ATOM	657		2 TH	R A	83		.00 34.35	A
MOTA	658			RA			.00 32.84 .00 33.97	A A
MOTA	659			RA			.00 33.97	A
ATOM ATOM	660 661			N I			.00 34.66	A
202 011		_ ~			- ••			

ATOM	662	СВ	asn	A	84	61.634	-0.252	6.069	1.00 36.13	A
ATOM	663	CG	ASN		84	62.337	-1.045	7.132	1.00 37.22	A
MOTA	664	OD1	asn	A	84	61.809	-1.241	8.220	1.00 39.34	A
MOTA	665	ND2	asn	A	84	63.548	-1.497	6.830	1.00 38.89	A
MOTA	666	C	asn	A	84	59.549	0.267	4.881	1.00 35.51	A
ATOM	667	0	asn		84	59.961	0.343	3.724	1.00 38.89	A
ATOM	668	N	GLΰ		85	58.546	1.004	5.344	1.00 34.17	A
ATOM	669	CA	GLU		85	57.890	2.001	4.507	1.00 32.82 1.00 36.55	A A
ATOM	670	CB	GLU		85	56.427 55.523	2.183 0.993	4.921 4.645	1.00 38.33	A
ATOM	671	CG	GLU GLU		85 85	55.271	0.782	3.167	1.00 46.65	A
MOTA	672	CD	GLU		85	54.829	1.741	2.494	1.00 49.22	A
ATOM ATOM	673 674		GLU		85	55.508	-0.345	2.679	1.00 48.74	A
ATOM	675	C	GFA		85	58.624	3.328	4.701	1.00 30.10	A
MOTA	676	ŏ	GLU		85	59.489	3.453	5.571	1.00 27.29	A
ATOM	677	N	VAL		86	58.274	4.308	3.878	1.00 28.67	A
ATOM	678	CA	VAL	A	86	58.849	5.641	3.951	1.00 27.33	A
ATOM	679	CB	VAL	A	86	59.146	6.202	2.539	1.00 27.74	A
MOTA	680	CG1	VAL	A	86	59.688	7.637	2.640	1.00 22.06	A
ATOM	681	CG2	VAL		86	60.139	5.289	1.815	1.00 25.30	A
ATOM	682	С	VAL		86	57.786	6.519	4.614	1.00 27.98	A A
ATOM	683	0	VAL		86	56.685	6.671	4.086 5.784	1.00 28.76 1.00 27.39	A
ATOM	684	N	PRO		87	58.095	7.098 6.861	6.644	1.00 26.00	A
ATOM	685	CD	PRO		87	59.268 57.106	7.949	6.458	1.00 28.38	A
ATOM	686	CA	PRO		87 87	57.611	7.989	7.899	1.00 26.97	A
MOTA	687	CB	PRO		87	59.099	7.915	7.727	1.00 27.97	A
ATOM ATOM	688 689	C	PRO		87	56.963	9.341	5.848	1.00 30.15	A
MOTA	690	o	PRO		87	57.902	9.871	5.245	1.00 31.62	A
MOTA	691	N	GLU		88	55.778	9.922	6.004	1.00 29.70	A
ATOM	692	CA	GLU		88	55.489	11.252	5.481	1.00 29.65	A
ATOM	693	CB	GLU		88	54.173	11.229	4.699	1.00 32.09	A
ATOM	694	CG	GLU	A	88	54.038	12.330	3.655	1.00 38.40	A
MOTA	695	CD	GLU	Α	88	52.790	12.172	2.792	1.00 41.07	A
ATOM	696		GLU		88	51.675	12.411	3.303	1.00 42.35	A
ATOM	697	OE2	GLU		88	52.925	11.800	1.604	1.00 43.46	A
MOTA	698	С	GLU		88	55.385	12.191	6.680	1.00 27.98	A A
MOTA	699	0	GLU		88	54.588	11.954	7.597	1.00 26.16 1.00 23.90	A
MOTA	700	N	VAI		89	56.187	13.253	6.672 7.788	1.00 23.90	A
ATOM	701	CA	VAI		89	56.201 57.637	14.194 14.358	8.333	1.00 18.36	A
MOTA	702	CB	IAV IAV .		89 89	57.639	15.295	9.534	1.00 17.11	A
ATOM ATOM	703 704		VAI		89	58.204	12.990	8.719	1.00 16.77	A
MOTA	705	C	VAI		89	55.626	15.575	7.483	1.00 21.60	A
MOTA	706	ō	VAI		89	55.859	16.143	6.420	1.00 21.72	A
ATOM	707	N	THE		90	54.886	16.115	8.444	1.00 21.28	A
MOTA	708	CA	THE	A S	90	54.269	17.425	8.301	1.00 20.62	A
ATOM	709	CB	THI	R A	90	52.813	17.303	7.823	1.00 21.90	A
MOTA	710		THI		90	52.770	16.537	6.613	1.00 26.43	A A
MOTA	711		THI		90	52.220	18.678	7.558	1.00 23.70 1.00 21.08	A
ATOM	712	C		R A	90	54.264	18.153 17.578	9.639 10.667	1.00 20.41	A
ATOM	713	0		R A	90	53.887 54.670	19.423	9.618	1.00 19.24	A
ATOM	714 715	N CA		L A L A	91 91	54.712	20.243	10.822	1.00 19.55	A
MOTA MOTA	716	CB		LΑ	91	56.149	20.739	11.102	1.00 19.97	A
ATOM	717		l VA			56.167	21.629	12.338	1.00 16.82	A
ATOM	718		2 VA			57.072	19.547	11.280	1.00 17.43	A
ATOM	719	C		LΑ		53.789	21.452	10.703	1.00 19.10	A
MOTA	720	0	VA	L A	91	53.735	22.108	9.666	1.00 20.59	A
ATOM	721	N	PH	ΕA		53.059	21.739	11.772	1.00 18.65	A
MOTA	722	CA		E A		52.146	22.870	11.785	1.00 19.10	A A
MOTA	723			E A		50.853	22.516	11.030	1.00 18.89	A
MOTA	724			E A		50.176 49.165	21.264	11.525 12.480	1.00 16.16 1.00 16.77	A
ATOM	725		1 PH			50.561		11.047		A
MOTA MOTA	726		2 PH 1 PH			48.543		12.955		A
MOTA	727 728		1 PH 2 PH			49.954		11.511		A
ATOM	728			EA		48.936		12.471		A
ATOM	730			E A		51.844		13.229		A
ATOM	731			E A		52.055		14.134	1.00 19.64	A
MOTA	732			R A		51.365		13.445		A
MOTA	733		SE	R A	93	51.052		14.792		A
MOTA	734			RA		51.275		14.921		A A
MOTA	735	OG	SE	ir a	93	50.435	27.132	14.043	1.00 20.17	*

ATOM	736	С	SER A	93	49.618	24.554	15.172	1.00 19.04	A
ATOM	737	ō	SER A	93	48.748	24.417	14.316	1.00 17.44	A
ATOM	738	N	LYS A	94	49.390	24.418	16.472	1.00 20.26	A
ATOM	739	CA	LYS A	94	48.077	24.108	17.010	1.00 21.70	A
ATOM	740	CB	LYS A	94	48.227	23.670	18.464	1.00 22.45	A
ATOM	741	CG	LYS A	94	46.938	23.273	19.139	1.00 24.42	A
ATOM	742	CD	LYS A	94	47.189	22.867	20.587	1.00 25.48	A
ATOM	743	CE	LYS A	94	45.881	22.548	21.297	1.00 25.73	A
		NZ	LYS A	94	45.122	21.533	20.517	1.00 26.34	A
ATOM	744	C	LYS A	94	47.169	25.340	16.921	1.00 23.44	A
ATOM	745 746	Ö	LYS A	94	45.984	25.235	16.598	1.00 20.95	A
ATOM		И	SER A	95	47.742	26.505	17.212	1.00 24.82	A
MOTA	747	CA	SER A	95	47.013	27.769	17.172	1.00 27.69	A
MOTA MOTA	748 749	CB	SER A	95	46.969	28.408	18.565	1.00 26.33	A ·
ATOM	750	OG	SER A	95	46.202	27.635	19.468	1.00 32.56	A
ATOM	751	C	SER A	95	47.688	28.747	16.219	1.00 27.36	A
MOTA	752	ō	SER A	95	48.824	28.529	15.797	1.00 27.94	A
MOTA	753	И	PRO A	96	46.985	29.830	15.849	1.00 27.27	A
MOTA	754	CD.	PRO A	96	45.611	30.232	16.193	1.00 28.85	A
ATOM	755	CA	PRO A	96	47.606	30.801	14.946	1.00 26.90	A
MOTA	756	СВ	PRO A	96	46.471	31.788	14.663	1.00 28.13	A
ATOM	757	CG	PRO A	96	45.634	31.719	15.907	1.00 28.36	A
ATOM	758	C	PRO A	96	48.786	31.421	15.700	1.00 24.92	A
ATOM	759	ō	PRO A	96	48.757	31.556	16.925	1.00 24.65	A
ATOM	760	N	VAL A	97	49.828	31.786	14.973	1.00 24.24	A
ATOM	761	CA	VAL A	97	51.016	32.332	15.601	1.00 25.15	A
ATOM	762	СВ	VAL A	97	52.261	32.087	14.715	1.00 26.78	A
ATOM	763		VAL A	97	53.531	32.372	15.508	1.00 26.15	A
ATOM	764		VAL A	97	52.255	30.659	14.198	1.00 26.15	A
ATOM	765	C	VAL A	97	50.935	33.820	15.920	1.00 25.62	A
ATOM	766	0	VAL A	97	50.624	34.638	15.054	1.00 25.01	A
ATOM	767	N	THR A	98	51.207	34.157	17.175	1.00 24.46	A
ATOM	768	CA	THR A	98	51.212	35.542	17.627	1.00 25.36	A
ATOM	769	CB	THR A	98	49.835	35.941	18.283	1.00 25.29	A
ATOM	770	OG1	THR A	98	50.030	37.008	19.217	1.00 30.50	A
MOTA	771	CG2	THR A	98	49.196	34.771	18.985	1.00 29.80	A
ATOM	772	C	THR A	98	52.382	35.678	18.605	1.00 24.87	A
ATOM	773	0	THR A	98	52.499	34.902	19.554	1.00 23.01	A
ATOM	774	N	LEU A	99	53.273	36.634	18.344	1.00 25.94	A
ATOM	775	CA	LEU A	99	54.445	36.843	19.198	1.00 28.02	A
ATOM	776	CB	TEA Y	99	55.194	38.114	18.797	1.00 31.12	A
ATOM	777	CG	LEU A	99	55.950	38.211	17.469	1.00 35.44	A
MOTA	778	CD1	LEU A	99	56.650	39.577	17.416	1.00 35.45	A
MOTA	779	CD2	LEU A	99	56.970	37.087	17.341	1.00 35.62	A
ATOM	780	С	TEA Y	99	54.135	36.932	20.689	1.00 27.10	A
MOTA	781	0	TEG Y		53.201	37.616	21.097	1.00 25.34	A
MOTA	782	N	GLY A		54.935	36.233	21.492	1.00 26.71	A
MOTA	783	CA	GLY A		54.762	36.253	22.935	1.00 26.48	A
MOTA	784	C	GLY A		53.635	35.398	23.479	1.00 26.32	A
MOTA	785	0	GLY A		53.428	35.323	24.695	1.00 25.37	A
MOTA	786	N	GLN A		52.913	34.734	22.585	1.00 25.16	A
ATOM	787	CA	GLN A		51.796	33.896	22.999	1.00 25.74	A
ATOM	788	CB	GLN A		50.573	34.219	22.143	1.00 28.06	A A
MOTA	789	CG	GLN A		49.258	33.911	22.814 24.162	1.00 30.50 1.00 32.88	A
MOTA	790	CD	GLN A		49.123	34.599 35.820		1.00 30.83	Ā
MOTA	791		L GLN A		48.953		24.251	1.00 33.04	A
ATOM	792		GLN A		49.202	33.813 32.409	25.221 22.901	1.00 33.04	A
ATOM	793	С	GLN A		52.117 52.280	31.881	21.807	1.00 24.25	A
MOTA	794	0	GLN A		52.199	31.715	24.051	1.00 22.08	A
MOTA	795	И	PRO P		51.959	32.244	25.410	1.00 22.41	A
MOTA	796	CD	PRO P		52.500	30.278	24.096	1.00 21.37	A
MOTA	797	CA			52.136	29.898	25.526	1.00 21.61	A
MOTA	798	CB	PRO P		52.521	31.147	26.297	1.00 21.90	A
MOTA	799	CG C	PRO P		51.706	29.480	23.068	1.00 21.30	A
MOTA MOTA	800	0	PRO A		50.496	29.644	22.947	1.00 21.93	A
ATOM	801 802		ASN A		52.396	28.618	22.327	1.00 18.86	A
ATOM	803	CA			51.749	27.802	21.305		A
ATOM	804		ASN A		52.040	28.379	19.913		A
ATOM	805				50.899	28.162	18.929		A
MOTA	806		1 ASN A		50.348	27.060	18.808		A
MOTA	807		2 ASN A		50.549	29.223	18.204		A
ATOM	808		ASN I		52.281	26.370	21.385		A
ATOM	809		ASN I		53.000	26.012	22.310		A
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MOTA	810		ILE A		51.918	25.565	20.397	1.00 15.80	A
MOTA	811		ILE A		52.335	24.177	20.328	1.00 13.66	A
MOTA	812	CB	ILE A		51.255 51.589	23.235 21.792	20.888	1.00 15.40 1.00 13.82	A A
ATOM ATOM	813 814		ILE A		51.132	23.421	22.400	1.00 17.40	A
MOTA	815		ILE A		50.129	22.494	23.047	1.00 18.65	A
ATOM	816	C	ILE A	104	52.588	23.775	18.896	1.00 14.36	A
MOTA	817	0	ILE A		51.716	23.924	18.052	1.00 16.86	A
ATOM	818	N	LEU A		53.785	23.272	18.616 17.272	1.00 15.67 1.00 15.52	A A
ATOM ATOM	819 820	CA CB	LEU A		54.090 55.568	22.822 22.978	16.940	1.00 15.73	A
ATOM	821	CG	LEU A		56.058	24.391	16.649	1.00 20.75	A
ATOM	822	CD1	LEU A	105	57.400	24.298	15.919	1.00 20.19	A
ATOM	823		LEU A		55.030	25.141	15.791	1.00 21.31	A
ATOM	824	C	LEU A		53.709 53.968	21.362 20.589	17.202 18.133	1.00 15.97 1.00 14.11	A A
ATOM ATOM	825 826	O N	ILE A		53.908	20.993	16.099	1.00 14.11	A
ATOM	827	CA	ILE A		52.643	19.630	15.903	1.00 15.40	A
ATOM	828	CB	ILE A	106	51.122	19.576	15.636	1.00 15.11	A
MOTA	829		ILE A		50.661	18.135	15.592	1.00 12.46	A
MOTA	830		ILE A		50.380 48.862	20.354	16.734 16.565	1.00 15.51 1.00 12.83	A A
ATOM ATOM	831 832	CDI	ILE A		53.381	19.011	14.725	1.00 16.48	A
ATOM	833	ō	ILE A		53.484	19.607	13.651	1.00 17.37	A
ATOM	834	N	CYS A	107	53.900	17.811	14.944	1.00 17.86	A
MOTA	835	CA	CYS A		54.621	17.083	13.917	1.00 18.32	A
MOTA	836	C	CYS A		53.886 53.846	15.776 14.909	13.663 14.533	1.00 18.29 1.00 18.13	A A
ATOM ATOM	837 838	O CB	CYS A		56.041	16.792	14.382	1.00 19.33	A
ATOM	839	SG	CYS A		57.029	15.889	13.158	1.00 25.82	A
MOTA	840	N	LEU A	108	53.304	15.649	12.472	1.00 17.89	A
ATOM	841	CA	LEU A		52.556	14.456	12.088	1.00 18.82	A A
ATOM	842	CB.	LEU A	•	51.330 50.129	14.850 13.900	11.252 11.053	1.00 20.17 1.00 21.48	A
MOTA MOTA	843 844		LEU A		49.623	14.049	9.624	1.00 20.62	A
ATOM	845		LEU A		50.493	12.458	11.316	1.00 18.40	A
MOTA	846	C	LEU A	108	.53.445	13.538	11.252	1.00 19.49	A
ATOM	847	0	LEU A	•	53.841	13.892	10.144	1.00 20.39 1.00 18.45	A A
ATOM ATOM	848 849	N CA	VAL A		53.760 54.586	12.368 11.398	11.789 11.087	1.00 19.04	A
ATOM	850	CB	VAL A		55.665	10.805	12.042	1.00 18.71	A
ATOM	851		VAL A		56.626	9.923	11.279	1.00 15.16	A
MOTA	852		VAL A		56.431	11.949	12.729	1.00 17.68	A
MOTA	853	C	VAL A		53.611	10.322 9.516	10.606 11.393	1.00 20.50 1.00 21.55	A A
ATOM ATOM	854 855	N O	VAL A		53.115 53.326	10.337	9.308	1.00 21.50	A
MOTA	856	CA	ASP A		52.376	9.407	8.700	1.00 21.95	A
MOTA	857	СВ	ASP A	A 110	51.493	10.165	7.701	1.00 22.25	A
ATOM	858	CG	ASP A		50.084	9.612	7.622	1.00 24.20	A
MOTA	859		ASP A		49.874 49.182	8.435 10.356	7.989 7.182	1.00 23.87 1.00 25.94	A A
MOTA MOTA	860 861	C	ASP A		53.059	8.240	7.985	1.00 21.53	A
ATOM	862	0	ASP A		54.273	8.254	7.782	1.00 18.80	A
MOTA	863	N		A 111	52.254	7.245	7.603	1.00 23.78	A
MOTA	864	CA		A 111 A 111	52.706 53.046	6.037 6.360	6.900 5.437	1.00 23.32 1.00 24.67	A A
MOTA MOTA	865 866	CB CG		A 111 A 111	53.181	5.102	4.575	1.00 31.76	A
ATOM	867		ASN A		52.291	4.240	4.567	1.00 31.05	A
MOTA	868	ND2	ASN 3		54.292	4.994	3.842	1.00 29.09	A
ATOM	869	C		A 111	53.905	5.389	7.587	1.00 23.68 1.00 22.88	A A
MOTA	870	N O		A 111 A 112	54.953 53.738	5.156 5.090	6.976 8.868	1.00 22.00	Ā
ATOM ATOM	871 872	CA		A 112	54.797	4.473	9.646	1.00 20.73	A
ATOM	873	CB	ILE :	A 112	54.791	4.967	11.108	1.00 20.13	A
MOTA	874		ILE		55.979	4.363	11.864	1.00 15.53	A
MOTA	875		ILE .		54.833	6.495 7.058	11.158 12.575	1.00 19.14 1.00 20.42	A A
ATOM ATOM	876 877	CD3	ILE .	A 112 A 112	54.671 54.658	2.960	9.699	1.00 20.42	A
ATOM	878	0		A 112	53.605	2.436	10.054	1.00 22.65	A
ATOM	879	N	PHE	A 113	55.732	2.266	9.343	1.00 21.37	A
ATOM	880	CA		A 113	55.769	0.819	9.412	1.00 21.74	A A
MOTA	881	CB		A 113	54.742 54.451	0.167 -1.252	8.483 8.850	1.00 21.64 1.00 21.22	A
MOTA MOTA	882 883	CCC:	PHE 1	A 113 A 113	53.528	-1.543	9.856	1.00 20.25	A
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ATOM	884	CD2	PHE A	113	55.183	-2.296	8.285	1.00 20.76	A
ATOM	885	CE1	PHE A	113	53.341	-2.848	10.302	1.00 19.85	A
ATOM	886	CE2	PHE A	113	55.008	-3.607	8.721	1.00 20.75	A
ATOM	887	CZ	PHE A	113	54.086	-3.887	9.735	1.00 21.24	A
ATOM	888	C	PHE A	113	57.157	0.329	9.042	1.00 21.21	A
MOTA	889	0	PHE A	. 113	57.700	0.719	8.011	1.00 19.97	A
MOTA	890	N	PRO A	114	57.765	-0.509	9.893	1.00 22.22	A
ATOM	891	СÐ	PRO A	114	59.118	-1.018	9.614	1.00 22.88	A
MOTA	892	CA	PRO A	114	57.263	-1.040	11.170	1.00 23.38	A
ATOM	893	CB	PRO A	114	58.340	-2.045	11.571	1.00 23.68	A
ATOM	894	CG	PRO A	114	59.592	-1.435	10.984	1.00 23.26	A
MOTA	895	C	PRO A	114	57.078	0.059	12.221	1.00 24.33	A
ATOM	896	0	PRO A	114	57.571	1.174	12.054	1.00 24.35	A
ATOM	897	N	PRO A	. 115	56.363	-0.247	13.319	1.00 24.59	A
ATOM	898	CD	PRO A		55.579	-1.472	13.567	1.00 22.60	A
MOTA	899	CA	PRO A		56.135	0.751	14.372	1.00 23.79	A
MOTA	900	CB	PRO A		54.923	0.194	15.107	1.00 23.96	A
MOTA	901	CG	PRO A		55.129	-1.291	14.998	1.00 23.45	A
ATOM	902	C	PRO A		57.337	0.996	15.289	1.00 24.97	A
ATOM	903	0	PRO A		57.322	0.670	16.482	1.00 23.11	A
ATOM	904	N	VAL A		58.380	1.573	14.705	1.00 24.77	A
ATOM	905	CA	VAL A		59.607	1.902	15.423	1.00 24.05	A
ATOM	906	СВ	VALA		60.733	0.881	15.135	1.00 26.45	A
ATOM	907		VAL A		61.977	1.250	15.933	1.00 24.89	A
ATOM	908		VAL A		60.267	-0.539	15.470	1.00 26.43	A
ATOM	909	C	VAL A		60.043	3.254	14.875	1.00 24.47	A
ATOM	910	0	VAL A		60.340	3.381	13.684	1.00 23.94 1.00 22.43	A A
ATOM	911	N	VAL A		60.088	4.269 5.577	15.728 15.239	1.00 22.43	A
ATOM	912	CA			60.472 59.247	6.277	14.565	1.00 22.18	A
ATOM	913 914	CB	VAL A		58.276	6.807	15.631	1.00 17.87	A
ATOM ATOM	915		VAL A		59.710	7.387	13.653	1.00 19.98	A
ATOM	916	C	VAL A		61.035	6.484	16.326	1.00 23.40	A
ATOM	917		VAL A		60.743	6.323	17.512	1.00 22.77	A
ATOM	918	N	ASN A		61.868	7.427	15.909	1.00 24.87	A
ATOM	919	CA	ASN A		62.434	8.398	16.833	1.00 25.96	A
ATOM	920	СВ	ASN A		63.970	8.341	16.858	1.00 29.36	A
ATOM	921	CG	ASN A		64,506	7.213	17.728	1.00 31.24	A
ATOM	922		ASN A		63.885	6.833	18.722	1.00 34.20	A
MOTA	923		ASN A		65.679	6.694	17.374	1.00 34.04	A
ATOM	924	C	ASN A	118	61.989	9.746	16.312	1.00 24.87	A
ATOM	925	0	ASN A	118	62.298	10.112	15.177	1.00 26.17	A
ATOM	926	N	ILE A	119	61.229	10.468	17.122	1.00 23.82	A
MOTA	927	CA	ILE A	119	60.774	11.793	16.727	1.00 23.07	A
MOTA	928	CB	ILE A	119	59.231	11.892	16.711	1.00 22.65	A
MOTA	929	CG2	ILE A	1119	58.797	13.197	16.051	1.00 18.01	A
MOTA	930		ILE A		58.642	10.716	15.936	1.00 21.02	A
MOTA	931		ILE A		57.135	10.714	15.921	1.00 21.88	A
ATOM	932	С	ILE A		61.323	12.771	17.754	1.00 22.76	A
ATOM	933	0	ILE A		61.013	12.680	18.940	1.00 22.92	A
ATOM	934	N	THR A	1 120	62.162	13.691	17.303	1.00 23.11	A
ATOM	935	CA	THR A		62.737	14.673	18.205	1.00 23.65	A
MOTA	936	CB	THR A		64.216	14.363	18.495	1.00 25.23	A
ATOM	937		THR A		64.921	14.199	17.258	1.00 26.55	A
ATOM	938		THR A		64.335	13.081	19.331	1.00 23.93	A
ATOM	939	C		A 120	62.622 62.437	16.064	17.616	1.00 23.20 1.00 23.15	A A
ATOM	940	0		A 120		16.232 17.069	16.412	1.00 23.13	A
ATOM	941	N		A 121 A 121	62.725 62.619	18.432	18.470 17.998	1.00 22.34	A
MOTA	942	CA CB		A 121	61.563	19.196	18.791	1.00 19.43	A
MOTA	943	CG		A 121	60.173	18.679	18.616	1.00 18.76	A
MOTA MOTA	944 945		TRP		59.191	19.179	17.703	1.00 19.96	A
ATOM	946		TRP		58.002	18.454	17.931	1.00 18.06	A
ATOM	947		TRP		59.200	20.178	16.715	1.00 16.07	A
ATOM	948		TRP		59.567	17.694	19.330	1.00 18.18	A
ATOM	949		TRP		58.261	17.553	18.929	1.00 19.21	A
MOTA	950		TRP		56.827	18.694	17.210	1.00 16.20	A
ATOM	951		TRP		58.036	20.419	16.000	1.00 16.43	A
ATOM	952		TRP		56.864	19.679	16.252	1.00 17.37	A
MOTA	953	C		A 121	63.927	19.178	18.097	1.00 22.88	A
ATOM	954	0		A 121	64.743	18.937	18.992	1.00 22.75	A
ATOM	955	N	LEU :	A 122	64.109	20.100	17.164	1.00 23.24	A
ATOM	956	CA		A 122	65.291	20.930	17.136	1.00 22.66	A
MOTA	957	СВ	LEU .	A 122	66.094	20.699	15.850	1.00 23.05	A
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MOTA	958	CG	LEU A 122	66.638	19.293	15.563	1.00 22.23	A
MOTA	959		LEU A 122	67.404	19.326	14.253	1.00 20.93	A
ATOM ATOM	960 961	CD2	LEU A 122 LEU A 122	67.542 64.837	18.830 22.376	16.700 17.186	1.00 20.21 1.00 23.52	A A
ATOM	962	ō	LEU A 122	63.830	22.752	16.572	1.00 21.74	A
ATOM	963	N	SER A 123	65.579	23.174	17.945	1.00 23.69	A
ATOM	964	CA	SER A 123	65.330	24.597	18.063	1.00 24.10	A
ATOM ATOM	965 966	CB OG	SER A 123 SER A 123	64.998 64.735	24.983 26.373	19.504 19.591	1.00 25.22 1.00 25.55	A A
ATOM	967	C	SER A 123	66.664	25.200	17.650	1.00 24.79	A
ATOM	968	0	SER A 123	67.670	25.014	18.335	1.00 23.07	A
ATOM	969	N	ASN A 124	66.666	25.903	16.521	1.00 25.02	A
ATOM	970 971	CA CB	ASN A 124 ASN A 124	67.880 68.351	26.513 27.676	15.986 16.868	1.00 25.63 1.00 24.46	A A
ATOM ATOM	972	CG	ASN A 124	67.376	28.839	16.873	1.00 25.33	A
ATOM	973		ASN A 124	66.636	29.056	15.907	1.00 26.04	A
ATOM	974		ASN A 124	67.381	29.606	17.956	1.00 21.77 1.00 26.53	A A
MOTA MOTA	975 976	C 0	ASN A 124 ASN A 124	69.006 70.132	25.487 25.706	15.838 16.301	1.00 26.36	A
ATOM	977	И	GLY A 125	68.684	24.361	15.205	1.00 24.78	A
ATOM	978	CA	GLY A 125	69.669	23.326	14.964	1.00 26.09	A
ATOM	979	C	GLY A 125	70.030	22.377	16.089	1.00 27.35	A A
ATOM ATOM	980 981	O N	GLY A 125 HIS A 126	70.728 69.566	21.395 22.645	15.846 17.307	1.00 28.21 1.00 28.65	A
ATOM	982	CA	HIS A 126	69.889	21.774	18.430	1.00 30.12	A
ATOM	983	СВ	HIS A 126	70.816	22.507	19.408	1.00 32.68	A
MOTA	984	CG	HIS A 126	70.226	23.750	19.996	1.00 35.25	A
MOTA	985		HIS A 126 HIS A 126	70.296 69.475	25.044 23.743	19.601 21.151	1.00 36.90 1.00 35.93	A A
ATOM ATOM	986 987		HIS A 126	69.110	24.979	21.445	1.00 36.88	A
ATOM	988		HIS A 126	69.595	25.788	20.520	1.00 36.73	A
MOTA	989	С	HIS A 126	68.661	21.220	19.149	1.00 30.87	A
ATOM	990	0	HIS A 126	67.634 68.789	21.889 19.990	19.270 19.635	1.00 31.49 1.00 30.93	A A
ATOM ATOM	991 992	n Ca	SER A 127 SER A 127	67.697	19.286	20.302	1.00 33.08	A
ATOM	993	СВ	SER A 127	68.165	17.889	20.714	1.00 33.91	A
ATOM	994	OG	SER A 127	69.231	17.979	21.645	1.00 38.34	A
ATOM	995	C	SER A 127	67.050	19.971	21.501 22.288	1.00 32.98 1.00 34.83	A A
MOTA MOTA	996 997	N O	SER A 127 VAL A 128	67.708 65.743	20.654 19.770	21.624	1.00 32.42	A
ATOM	998	CA	VAL A 128	64.960	20.325	22.716	1.00 31.29	A
MOTA	999	CB	VAL A 128	63.645	20.921	22.202	1.00 30.48	A
MOTA	1000		VAL A 128	62.856	21.520	23.358 21.142	1.00 27.06 1.00 28.52	A A
ATOM ATOM	1001	CG2	VAL A 128 VAL A 128	63.937 64.645	21.970 19.183	23.669	1.00 28.32	A
MOTA	1003	ō	VAL A 128	64.275	18.093	23.237	1.00 32.80	A
MOTA	1004	N	THR A 129	64.786	19.437	24.965	1.00 33.30	A
MOTA	1005	CA	THR A 129	64.546	18.411	25.981 26.966	1.00 33.70 1.00 34.52	A A
ATOM ATOM	1006 1007	CB OG1	THR A 129 THR A 129	65.740 65.969	18.344 19.643	27.528	1.00 34.32	A
ATOM	1008	CG2		67.006	17.898	26.245	1.00 34.60	A
MOTA	1009	C	THR A 129	63.257	18.591	26.791	1.00 32.08	A
MOTA	1010	0	THR A 129	62.645	17.615	27.220 26.993	1.00 34.04 1.00 28.85	A A
MOTA MOTA	1011	N CA	GLU A 130 GLU A 130	62.843 61.639	19.835 20.119	27.762	1.00 26.09	A
MOTA	1013	CB	GLU A 130	61.926	21.236	28.770	1.00 28.58	A
MOTA	1014	CG	GLU A 130	62.962	20.894	29.822	1.00 32.87	A
ATOM	1015	CD	GLU A 130	62.592	19.654	30.609 30.907	1.00 35.34 1.00 37.85	A A
ATOM ATOM	1016 1017		GLU A 130	61.392 63.501	19.475 18.865	30.941	1.00 37.83	A
ATOM	1018	C	GLU A 130	60.451	20.534	26.893	1.00 23.53	A
ATOM	1019	0	GLU A 130	60.629	21.166	25.859	1.00 19.76	A
MOTA	1020	N	GLY A 131	59.243	20.188	27.334	1.00 21.13 1.00 20.14	A A
MOTA	1021 1022	CA C	GLY A 131 GLY A 131	58.046 57.693	20.563 19.684	26.601 25.421	1.00 20.14	A
MOTA MOTA	1022	0	GLY A 131	56.989	20.109	24.507	1.00 20.11	A
ATOM	1024	N	VAL A 132	58.164	18.447	25.444	1.00 18.28	A
MOTA	1025	CA	VAL A 132	57.899			1.00 20.08	A A
MOTA	1026	CB	VAL A 132 1 VAL A 132	59.230 58.946			1.00 20.35 1.00 22.11	A A
MOTA MOTA	1027 1028		2 VAL A 132	60.006			1.00 20.17	A
ATOM	1029	C	VAL A 132	57.027	16.340	24.786	1.00 20.06	A
MOTA	1030	0	VAL A 132	57.194			1.00 18.65	A N
MOTA	1031	N	SER A 133	56.094	15.948	23.925	1.00 17.90	A

MOTA	1032	CA	SER A 133	55.238	14.802	24.215	1.00 18.16	A
ATOM	1033	СВ	SER A 133	54.045	15.206	25.094	1.00 18.24	A
ATOM	1034	og	SER A 133 SER A 133	53.202 54.738	16.143 14.200	24.440 22.914	1.00 24.24 1.00 16.52	A A
ATOM ATOM	1035 1036	С О	SER A 133	54.736	14.794	21.843	1.00 16.18	A
ATOM	1037	N	GLU A 134	54.166	13.009	22.996	1.00 17.45	A
ATOM	1038	CA	GLU A 134	53.653	12.369	21.800	1.00 18.50	A
MOTA	1039	CB	GLU A 134	54.797	11.661	21.050	1.00 22.31	A
MOTA	1040	CG	GLU A 134	55.475	10.513	21.801	1.00 24.62	A
ATOM	1041	CD	GLU A 134	56.610	9.859 8.680	20.992 21.254	1.00 28.65 1.00 29.58	A A
MOTA MOTA	1042 1043		GLU A 134 GLU A 134	56.932 57.188	10.521	20.099	1.00 27.96	A
ATOM	1044	C	GLU A 134	52.523	11.389	22.087	1.00 18.44	A
ATOM	1045	ō	GLU A 134	52.279	11.003	23.234	1.00 17.30	A
MOTA	1046	N	THR A 135	51.824	11.008	21.027	1.00 16.71	A
ATOM	1047	CA	THR A 135	50.733	10.059	21.119	1.00 15.49 1.00 16.16	A A
ATOM	1048	CB	THR A 135 THR A 135	49.738 50.369	10.246 9.867	19.967 18.731	1.00 16.02	A
ATOM ATOM	1049 1050		THR A 135	49.280	11.697	19.879	1.00 14.19	A
ATOM	1051	c	THR A 135	51.346	8.682	20.946	1.00 17.19	A
ATOM	1052	0	THR A 135	52.551	8.554	20.733	1.00 17.26	A
ATOM	1053	N	SER A 136	50.519	7.650	21.047	1.00 17.53	A
MOTA	1054	CA	SER A 136	51.001	6.297	20.818	1.00 15.92 1.00 16.85	A A
ATOM	1055	CB	SER A 136 SER A 136	50.035 49.756	5.266 5.532	21.416 22.781	1.00 18.22	A
MOTA MOTA	1056 1057	OG C	SER A 136	50.967	6.187	19.294		A
ATOM	1058	ō	SER A 136	50.715	7.169	18.596	1.00 17.25	A
MOTA	1059	N	PHE A 137	51.236	5.003	18.767	1.00 17.08	A
MOTA	1060	CA	PHE A 137	51.155	4.806	17.333	1.00 15.67	A
MOTA	1061	CB	PHE A 137	51.874	3.519	16.936	1.00 13.47 1.00 14.48	A A
ATOM	1062	CG	PHE A 137	53.363 54.037	3.628 4.255	16.951 15.907	1.00 15.82	A
ATOM ATOM	1063 1064		PHE A 137	54.100	3.112	18.010	1.00 15.21	A
MOTA	1065		PHE A 137	55.427	4.367	15.918	1.00 15.72	A
ATOM	1066	CE2		55.490	3.220	18.031	1.00 15.14	A
ATOM	1067	CZ	PHE A 137	56.152	3.848	16.983	1.00 14.35	A
ATOM	1068	C	PHE A 137	49.659	4.657	17.067 17.622	1.00 16.21 1.00 18.05	A A
MOTA	1069	N O	PHE A 137 LEU A 138	49.037 49.074	3.767 5.534	16.259	1.00 17.51	A
ATOM ATOM	1070 1071	CA	LEU A 138	47.648	5.433	15.953	1.00 19.20	A
ATOM	1072	CB	LEU A 138	47.017	6.822	15.800	1.00 20.80	A
MOTA	1073	CG	LEU A 138	46.809	7.688	17.044	1.00 23.47	A
MOTA	1074		LEU A 138	46.141	6.879	18.144	1.00 24.75	A A
ATOM	1075		LEU A 138	48.140 47.490	8.212 4.637	17.529 14.658	1.00 27.62 1.00 18.41	A
MOTA MOTA	1076 1077	C	LEU A 138 LEU A 138	48.218	4.862	13.698	1.00 16.16	A
MOTA	1077	N	SER A 139	46.530	3.716	14.630	1.00 18.51	A
ATOM	1079	CA	SER A 139	46.333	2.863	13.460	1.00 17.61	A
MOTA	1080	СВ	SER A 139	45.481	1.656	13.836	1.00 18.17	A
MOTA	1081	OG	SER A 139	44.134	2.036	14.040 12.216	1.00 20.80 1.00 17.44	A A
ATOM	1082	0	SER A 139 SER A 139	45.729 45.122	3.510 4.578	12.276	1.00 16.41	A
ATOM ATOM	1083 1084	71	LYS A 140	45.908	2.822	11.088	1.00 18.56	A
MOTA	1085	CA	LYS A 140	45.402	3.237	9.778	1.00 18.37	A
MOTA	1086	CB	LYS A 140	46.543	3.751	8.895	1.00 21.60	A
MOTA	1087	CG	LYS A 140	47.149	5.085	9.326	1.00 24.86 1.00 30.27	A A
ATOM	1088	CD	LYS A 140 LYS A 140	46.513 46.961	6.267 6.345			A
MOTA MOTA	1089 1090	CE NZ	LYS A 140	48.440	6.349			A
ATOM	1091	c	LYS A 140	44.773	2.012			A
ATOM	1092	0	LYS A 140	45.106				A
MOTA	1093		SER A 141	43.882				A
MOTA	1094			43.220				A A
MOTA	1095			42.047 42.490				A
ATOM ATOM	1096 1097		SER A 141	44.154				A
ATOM	1098		SER A 141	43.828		6.332		A
ATOM	1099		ASP A 142	45.311				A
MOTA	1100			46.234				A A
ATOM	1101			47.008 47.949				A
MOTA MOTA	1102 1103		1 ASP A 142	47.837				A
MOTA	1104		2 ASP A 142	48.799		4.354	1.00 28.43	A
MOTA	1105		ASP A 142	47.176	-0.752	6.368	1.00 20.11	A

MOTA	1106	0	ASP A 142	48.127	-1.416	5.946	1.00 19.21	A
MOTA	1107	N	HIS A 143	46.885	-0.626	7.659 8.706	1.00 18.99 1.00 17.27	A A
ATOM ATOM	1108 1109	CA CB	HIS A 143 HIS A 143	47.637 47.686	-1.295 -2.792	8.409	1.00 16.45	A
ATOM	1110	CG	HIS A 143	46.329	-3.396	8.190	1.00 18.33	A
ATOM	1111		HIS A 143	45.860	-4.211	7.213	1.00 17.59	A
ATOM	1112	ND1	HIS A 143	45.262	-3.151	9.032	1.00 15.97	A
ATOM	1113		HIS A 143	44.194	-3.786	8.580	1.00 19.46	A
ATOM	1114		HIS A 143	44.529	-4.436 -0.749	7.478 9.030	1.00 18.06 1.00 19.46	A A
ATOM ATOM	1115 1116	С 0	HIS A 143	49.019 49.812	-1.401	9.715	1.00 19.95	A
ATOM	1117	N	SER A 144	49.301	0.454	8.536	1.00 19.70	A
MOTA	1118	CA	SER A 144	50.542	1.141	8.852	1.00 20.18	A
MOTA	1119	CB	SER A 144	51.018	2.011	7.678	1.00 19.91	A
ATOM	1120	OG	SER A 144	50.099	3.044	7.364	1.00 23.64	A A
ATOM	1121	C	SER A 144 SER A 144	50.109 48.970	2.018 1.906	10.034	1.00 19.40 1.00 19.70	A
ATOM ATOM	1122 1123	N N	PHE A 145	50.986	2.883	10.525	1.00 16.99	A
ATOM	1124	CA	PHE A 145	50.614	3.728	11.649	1.00 16.06	A
ATOM	1125	СВ	PHE A 145	51.325	3.274	12.929	1.00 16.25	A
ATOM	1126	CG	PHE A 145	51.062	1.841	13.297	1.00 19.53	A
MOTA	1127		PHE A 145	51.754	0.807	12.672	1.00 20.17	A A
ATOM	1128		PHE A 145	50.114	1.522 -0.525	14.263 13.005	1.00 18.18 1.00 21.33	A
MOTA	1129	CE1	PHE A 145 PHE A 145	51.505 49.856	0.193	14.606	1.00 19.50	A
MOTA MOTA	1130 1131	CZ	PHE A 145	50.553	-0.831		1.00 20.23	A
ATOM	1132	c	PHE A 145	50.955	5.182	11.419	1.00 15.69	A
ATOM	1133	0	PHE A 145	51.548	5.538	10.404	1.00 16.69	A
MOTA	1134	N	PHE A 146	50.530	6.021	12.357	1.00 14.53 1.00 16.67	A A
MOTA	1135	CA	PHE A 146	50.869 49.841	7.429 8.279	12.332 11.552	1.00 16.57	A
ATOM	1136	CB	PHE A 146 PHE A 146	48.535	8.528	12.259	1.00 15.25	A
MOTA MOTA	1137 1138		PHE A 146	48.370	9.644	13.071	1.00 15.42	A
ATOM	1139		PHE A 146	47.433	7.708	12.019	1.00 16.06	A
ATOM	1140	CE1	PHE A 146	47.123	9.952	13.629	1.00 17.50	A
MOTA	1141	CE2		46.180	8.003	12.571	1.00 16.80 1.00 17.47	A A
MOTA	1142	CZ	PHE A 146	46.023	9.126 7.841	13.375 13.783	1.00 17.00	Ā
MOTA	1143	0	PHE A 146 PHE A 146	51.017 50.345	7.308	14.661	1.00 19.50	A
ATOM ATOM	1144 1145	N	LYS A 147	51.950	8.747	14.032	1.00 17.82	A
ATOM	1146	CA	LYS A 147	52.224	9.221	15.377	1.00 18.67	A
ATOM	1147	CB	LYS A 147	53.540	8.604	15.863	1.00 20.48	A
MOTA	1148	CG	LYS A 147	53.771	8.668	17.359	1.00 25.54 1.00 29.96	A A
MOTA	1149	CD	LYS A 147	54.822 54.835	7.645 7.417	17.774 19.282	1.00 30.05	A
MOTA MOTA	1150 1151	CE NZ	LYS A 147 LYS A 147	55.740	6.291	19.643	1.00 33.05	A
ATOM	1152	C	LYS A 147	52.315	10.743	15.338	1.00 17.25	A
ATOM	1153	0	LYS A 147	52.716	11.320	14.329	1.00 19.15	A
MOTA	1154	N	ILE A 148	51.932	11.391	16.428	1.00 15.47	A
MOTA	1155	CA	ILE A 148	.51.969	12.846	16.494 16.642	1.00 14.99 1.00 15.37	A A
MOTA	1156	CB	ILE A 148 2 ILE A 148	50.529 50.566	13.424 14.932	16.740	1.00 14.06	A
MOTA MOTA	1157 1158	CG:	1 ILE A 148	49.689	13.025	15.426	1.00 16.41	A
ATOM	1159		1 ILE A 148	48.223	13.325	15.550	1.00 18.61	A
MOTA	1160		ILE A 148	52.829	13.271	17.682	1.00 17.07	A
MOTA	1161		ILB A 148	52.721		18.772	1.00 15.61	A A
ATOM	1162		SER A 149	53.696 54.570	14.255 14.757	17.458 18.514	1.00 16.79 1.00 17.66	A
MOTA	1163			56.042		18.116		A
MOTA MOTA	1164 1165			56.900		19.190		A
ATOM	1166		SER A 149	54.239		18.763		A
MOTA	1167		SER A 149	53.854				A
ATOM	1168		TYR A 150	54.401				A A
MOTA	1169			54.085				A
MOTA	1170			52.893 51.679				A
MOTA MOTA	1171 1172		11R A 150	50.879				A
ATOM	1173		1 TYR A 150	49.733		19.340	1.00 18.32	A
MOTA	1174	CE	2 TYR A 150	51.313				A N
ATOM	1175		2 TYR A 150	50.176				A A
MOTA	1176			49.391				A
ATOM	1177		TYR A 150 TYR A 150	48.275 55.237				A
MOTA MOTA	1178 1179		TYR A 150	55.953				A

1180 N LEU A 151 55.409 20.029 20.649 1.00 17.01 ATOM ATOM 1181 CA LEU A 151 56.449 20.868 21.224 1.00 15.24 MOTA 1182 CB LEU A 151 57.540 21.182 20.197 1.00 16.33 58.487 22.335 20.575 1.00 16.27 CG LEU A 151 ATOM 1183 MOTA 1184 CD1 LEU A 151 59.402 21.906 21.706 1.00 17.13 CD2 LEU A 151 59.315 22.755 19.359 ATOM 1185 1.00 19.34 ATOM 1186 C LEU A 151 55.825 22.174 21.666 1.00 16.08 55.221 22.881 20.860 1.00 16.22 55.952 22.497 22.945 1.00 16.84 ATOM 1187 O LEU A 151 ATOM 1188 N THR A 152 A CA THR A 152 55.428 23.765 23.424 1.00 18.70 MOTA 1189 55.283 23.799 24.946 1.00 20.14 56.576 23.633 25.544 1.00 23.32 1190 CB THR A 152 ATOM A MOTA 1191 OG1 THR A 152 A CG2 THR A 152 54.355 22.694 25.419 1.00 18.36 ATOM 1192 ATOM 1193 С THR A 152 56.498 24.772 23.050 1.00 20.04 57.689 24.448 1.00 20.72 THR A 152 23.034 ATOM 1194 0 56.085 25.986 22.735 1.00 20.63 ATOM 1195 N LEU A 153 A CA LEU A 153 57.043 27.014 22.389 1.00 24.69 ATOM 1196 Α CB LEU A 153 57.579 26.794 MOTA 1197 20.960 1.00 24.19 56.716 26.942 19.694 55.303 26.451 19.959 CG LEU A 153 1.00 26.72 ATOM 1198 MOTA 1199 CD1 LEU A 153 1.00 27.32 ATOM 1200 CD2 LEU A 153 56.686 28.393 19.249 1.00 26.15 ATOM 1201 C LEU A 153 56.410 28.385 22.531 1.00 26.36 A LEU A 153 56.410 28.385 22.531 LEU A 153 55.180 28.511 22.597 1.00 29.59 ATOM 1202 n MOTA 1203 N LEU A 154 57.262 29.401 22.620 1.00 26.29 CA LEU A 154 56.830 30.787 22.729 1.00 26.89 ATOM 1204 CA LEU A 154 56.830 30.787 22.729 1.00 26.89 CB LEU A 154 57.459 31.444 23.965 1.00 26.94 MOTA 1205 CG LEU A 154 56.966 32.833 CD1 LEU A 154 55.507 32.755 24.407 1.00 28.58 MOTA 1206 MOTA 1207 24.864 1.00 24.43 CD2 LEU A 154 57.845 33.342 1208 25.549 1.00 27.14 ATOM 57.337 31.458 58.538 31.689 LEU A 154 21.456 1.00 28.94 MOTA 1209 C 21.304 1.00 30.73 MOTA 1210 0 LEU A 154 56.428 31.773 54.975 31.534 56.806 32.412 ATOM 1211 N PRO A 155 20.518 1.00 30.57 20.559 1.00 29.60 MOTA 1212 CD PRO A 155 CA PRO A 155 19.254 1.00 31.63 ATOM 1213 55.460 32.668 18.581 1.00 30.63 PRO A 155 ATOM 1214 CB 1215 PRO A 155 54.612 31.552 19.087 1.00 28.73 ATOM CG 19.370 1.00 33.58 57.639 33.688 MOTA 1216 C PRO A 155 57.322 34.593 20.136 1.00 33.98 58.706 33.741 18.586 1.00 35.79 PRO A 155 ATOM 1217 0 ATOM 1218 N SER A 156 1219 CA SER A 156 59.595 34.888 18.546 1.00 37.77 ATOM SER A 156 60.604 34.839 19.694 1.00 38.66 ATOM 1220 CB 59.955 34.966 SER A 156 20.949 1.00 44.00 ATOM 1221 OG 60.332 34.841 60.257 33.849 17.222 1.00 38.83 C SER A 156 ATOM 1222 ATOM 1223 0 SER A 156 16.492 1.00 38.36 61.042 35.915 ALA A 157 16.909 1.00 40.38 MOTA 1224 N 61.796 35.972 15.670 1.00 39.93 61.822 37.401 15.148 1.00 40.36 ATOM 1225 CA ALA A 157 CB ALA A 157 ATOM 1226 15.918 1.00 39.65 MOTA 1227 C ALA A 157 63.214 35.466 ALA A 157 64.058 35.504 15.021 1.00 39.72 MOTA 1228 0 63.463 34.984 ATOM 1229 N GLU A 158 17.135 1.00 39.12 64.784 34.480 17.517 1.00 40.24 65.082 34.808 18.988 1.00 44.21 1230 CA GLU A 158 ATOM ATOM 1231 CB GLU A 158 CG GLU A 158 ATOM 1232 65.426 36.268 19.287 1.00 50.31 64.204 37.174 19.356 1.00 55.36 64.353 38.351 19.765 1.00 55.75 1233 CD GLU A 158 ATOM OE1 GLU A 158 ATOM 1234 63.095 36.712 19.002 1.00 58.12 ATOM 1235 OE2 GLU A 158 MOTA 1236 С GLU A 158 65.005 32.979 17.303 1.00 38.02 66.130 32.493 17.419 1.00 36.30 GLU A 158 1237 0 MOTA 63.950 32.234 17.002 1.00 35.79 GLU A 159 MOTA 1238 N ATOM 1239 CA GLU A 159 64.136 30.807 16.805 1.00 35.02 Α GLU A 159 63.949 30.066 18.135 1.00 36.97 ATOM 1240 CB CG GLU A 159 62.699 30.439 18.891 1.00 41.68 MOTA 1241 20.323 1.00 44.82 62.717 29.933 MOTA 1242 CD GLU A 159 MOTA 1243 OE1 GLU A 159 62.819 28.705 20.527 1.00 46.62 1244 OE2 GLU A 159 62.631 30.767 21.248 1.00 47.25 ATOM 1245 C GLU A 159 63.277 30.162 15.735 1.00 32.21 MOTA 62.147 30.574 15.473 1.00 32.05 MOTA 1246 0 GLU A 159 29.147 15.107 1.00 29.55 ATOM 1247 N SER A 160 63.849 MOTA 1248 CA SER A 160 63.167 28.394 14.076 1.00 28.89 28.551 12.734 1.00 27.34 MOTA 1249 CB SER A 160 63.885 ATOM 1250 OG SER A 160 65.206 28.053 12.807 1.00 29.49 63.241 26.957 14.565 1.00 27.42 1251 C SER A 160 MOTA 64.092 26.628 15.392 1.00 25.45 ATOM 1252 0 SER A 160 62.359 26.101 14.066 1.00 24.73 ATOM 1253 N TYR A 161

MOTA	1254	CA	TYR	A	161	62.359	24.725	14.517	1.00 24.26	A
MOTA	1255	CB	TYR	A	161	61.172	24.480	15.451	1.00 23.50	A
MOTA	1256	CG	TYR			60.935	25.593	16.434	1.00 24.01	A
MOTA	1257		TYR			60.255	26.748	16.052	1.00 26.02	A
MOTA	1258		TYR			60.009	27.774	16.959	1.00 27.93	A
ATOM	1259		TYR			61.374	25.491	17.753	1.00 24.78	A
MOTA	1260		TYR			61.136	26.514	18.674	1.00 25.93	A
ATOM ATOM	1261 1262	CZ	TYR			60.450	27.650	18.270	1.00 27.56	A
ATOM	1263	C	TYR TYR			60.182 62.330	28.650	19.173	1.00 29.78	A
ATOM	1264	0	TYR			62.082	23.700 24.021	13.397 12.239	1.00 25.15 1.00 24.96	A
ATOM	1265	N	ASP			62.600	22.455	13.775	1.00 26.26	A A
MOTA	1266	CA	ASP			62.598	21.331	12.858	1.00 26.94	A
MOTA	1267	CB	ASP			64.007	21.014	12.356	1.00 30.11	A
ATOM	1268	CG	ASP	A	162	64.548	22.067	11.434	1.00 32.85	A
MOTA	1269	OD1	ASP	A	162	64.075	22.138	10.277	1.00 33.31	A
MOTA	1270	OD2	ASP	A	162	65.443	22.819	11.874	1.00 33.08	A
ATOM	1271	C	ASP			62.122	20.117	13.613	1.00 25.87	A
MOTA	1272	0	ASP			62.449	19.947	14.789	1.00 24.38	A
ATOM	1273	N	CYS			61.352	19.277	12.935	1.00 23.95	A
ATOM	1274	CA	CYS			60.914	18.027	13.530	1.00 24.46	A
MOTA	1275	C	CYS			61.916	17.043	12.938	1.00 22.46	A
ATOM	1276	O CD	CYS CYS			62.110	17.021	11.726	1.00 24.01	A
ATOM ATOM	1277 1278	CB SG	CYS			59.497 58.931	17.658 16.101	13.083	1.00 24.14	A
ATOM	1279	Ŋ	LYS			62.571	16.259	13.836 13.782	1.00 30.35 1.00 22.96	A A
ATOM	1280	CA	LYS			63.559	15.292	13.702	1.00 24.69	A
ATOM	1281	CB	LYS			64.867	15.450	14.089	1.00 27.54	Ā
ATOM	1282	CG	LYS			65.977	14.490	13.689	1.00 28.93	A
ATOM	1283	CD	LYS			67.179	14.643	14.622	1.00 32.03	A
ATOM	1284	CE	LYS			68.254	13.596	14.350	1.00 33.85	A
MOTA	1285	NZ	LYS	A	164	69.319	13.607	15.398	1.00 36.46	A
MOTA	1286	С	LYS	A	164	63.023	13.875	13.463	1.00 24.25	A
ATOM	1287	0	LYS			62.697	13.443	14.570	1.00 23.52	A
MOTA	1288	N	VAL			62.931	13.160	12.345	1.00 23.37	A
ATOM	1289	CA	VAL			62.415	11.797	12.344	1.00 24.06	A
ATOM	1290	СВ	VAL			61.174	11.682	11.408	1.00 23.45	A
MOTA	1291		VAL			60.657	10.248	11.382	1.00 18.80	A
ATOM ATOM	1292 1293	C	VAL VAL			60.078 63.457	12.632 10.772	11.878 11.903	1.00 22.37 1.00 25.04	A A
MOTA	1294	0	VAL			64.103	10.772	10.869	1.00 25.04	A
ATOM	1295	N	GLU			63.621	9.725	12.703	1.00 26.91	A
ATOM	1296	CA	GLU			64.556	8.648	12.383	1.00 28.84	A
MOTA	1297	СВ	GLU			65.554	8.424	13.523	1.00 30.71	A
ATOM	1298	CG	GLU			66.382	9.634	13.922	1.00 36.90	A
ATOM	1299	CD	GLŪ	A	166	67.247	9.356	15.147	1.00 39.97	A
MOTA	1300	0E1	GLU	A	166	67.466	10.286	15.954	1.00 43.02	A
MOTA	1301		GLU			67.714	8.206	15.301	1.00 43.24	A
MOTA	1302	C	GLU			63.739	7.369	12.183	1.00 28.96	A
ATOM	1303	0	GLU			62.975	6.971	13.067	1.00 27.40	A
ATOM ATOM	1304 1305	N CA	HIS HIS			63.910	6.728	11.029	1.00 29.87	A A
ATOM	1305	CB			167	63.189 61.838	5.496 5.833	10.713 10.084	1.00 30.70 1.00 30.90	A
ATOM	1307	CG	HIS			60.932	4.655	9.933	1.00 34.01	A
ATOM	1308		HIS			60.698	3.842	8.876	1.00 33.60	A
MOTA	1309		HIS			60.159	4.172	10.967	1.00 36.69	A
ATOM	1310		HIS			59.488	3.112	10.554	1.00 34.84	A
MOTA	1311	NE2	HIS	A	167	59.798	2.890	9.290	1.00 34.90	A
ATOM	1312	C	HIS	A	167	63.999	4.639	9.739	1.00 31.21	A
MOTA	1313	0			167	64.696	5.167	8.866	1.00 29.44	A
ATOM	1314	N			168	63.895	3.320	9.879	1.00 31.70	A
ATOM	1315	CA			168	64.625	2.402	9.006	1.00 31.76	A
MOTA	1316	CB			168	64.344	0.954	9.396	1.00 30.39	A
atom Atom	1317 1318	CG	TRP		168	64.735 64.115	0.650 -0.297	10.797 11.666	1.00 28.49 1.00 28.31	A A
MOTA	1319		TRP			64.837	-0.297	12.878	1.00 28.31	A
ATOM	1320		TRP			63.017	-1.157	11.538	1.00 26.47	A
ATOM	1321		TRP			65.778	1.184	11.491	1.00 28.32	A
MOTA	1322		TRP			65.849	0.627	12.744	1.00 28.98	A
ATOM	1323		TRP			64.498	-1.107	13.958	1.00 28.85	A
ATOM	1324		TRP			62.678	-1.970	12.608	1.00 27.57	A
MOTA	1325		TRP			63.418	-1.940	13.805	1.00 29.20	A
MOTA	1326	C			168	64.332	2.588	7.523	1.00 33.06	A
ATOM	1327	0	TKP	A	168	65.190	2.314	6.682	1.00 32.28	A

MOTA	1328	N	GLY A 1	69 6	3.126	3.049	7.202	1.00 34.81	A
ATOM	1329	CA	GLY A 1		2.760	3.263	5.810	1.00 35.23	A
ATOM	1330	c c	GLY A 1		3.267	4.588	5.266	1.00 37,25	A
ATOM	1331	ŏ	GLY A 1		2.907	4.992	4.162	1.00 37.65	A
ATOM	1332	N	LEU A 1		4.100	5.268	6.049	1.00 39.27	A
ATOM	1333	CA	LEU A 1		4.673	6.555	5.660	1.00 41.10	A
ATOM	1334	CB	LEU A 1		4.354	7.626	6.706	1.00 38.47	A
ATOM	1335	CG	LEU A 1		2.923	8.143	6.843	1.00 38.66	A
ATOM	1336		LEU A 1		2.790	8.919	8.142	1.00 37.48	A
			LEU A 1		2.572	9.017	5.653	1.00 37.45	A
MOTA	1337						5.556	1.00 43.62	A
ATOM	1338	C	LEU A 1		6.183	6.425	6.382	1.00 44.45	A
MOTA	1339	0			6.809	5.762			A
MOTA	1340	N	ASP A 1		6.764	7.066	4.545	1.00 46.98	A
ATOM	1341	CA	ASP A 1		8.211	7.036	4.350	1.00 48.99	
ATOM	1342	СВ	ASP A 1		8.602	7.810	3.086	1.00 51.12	A
MOTA	1343	CG	ASP A 1		7.735	7.466	1.895	1.00 53.30	A
ATOM	1344		ASP A 1		6.520	7.761	1.936	1.00 54.82	A
MOTA	1345		ASP A 1		8.271	6.903	0.917	1.00 54.86	A
MOTA	1346	С	ASP A 1		8.836	7.726	5.554	1.00 48.82	A
ATOM	1347	0	ASP A 1		9.437	7.093	6.420	1.00 48.88	A
ATOM	1348	N	LYS A 1		8.673	9.044	5.585	1.00 48.96	A
MOTA	1349	CA	LYS A 1		9.192	9.877	6.659	1.00 48.79	A
ATOM	1350	CB	LYS A 1			11.059	6.084	1.00 51.32	A
MOTA	1351	CG	LYS A 1			10.698	5.075	1.00 55.53	A
ATOM	1352	CD	LYS A 1			11.952	4.571	1.00 57.81	A
MOTA	1353	CE	LYS A 1		2.859	11.621	3.518	1.00 59.22	A
MOTA	1354	NZ	LYS A 1		3.912	10.702	4.038	1.00 58.32	A
MOTA	1355	C	LYS A 1	.72 6	7.990	10.419	7.420	1.00 46.36	A
MOTA	1356	0	LYS A 1		6.862	10.381	6.919	1.00 44.39	A
MOTA	1357	N	PRO A 1	.73 6	8.211	10.920	8.645	1.00 44.20	A
MOTA	1358	CD	PRO A 1		9.432	10.866	9.469	1.00 44.15	A
MOTA	1359	CA	PRO A 1	.73 6	7.089	11.462	9.410	1.00 42.74	A
ATOM	1360	CB	PRO A 1	.73 6	7.768	12.050	10.637	1.00 42.02	A
ATOM	1361	CG	PRO A 1	L73 6	8.887	11.080	10.872	1.00 44.25	A
MOTA	1362	C	PRO A 1	.73 €	6.369	12.517	8.578	1.00 41.09	A
ATOM	1363	0	PRO A 1	L73 €	7.002	13.309	7.877	1.00 39.67	A
MOTA	1364	N	LEU A 1	L74 6	5.044	12.502	8.636	1.00 39.80	A
MOTA	1365	CA	LEU A 1	L74 6	4.241	13.457	7.888	1.00 38.58	A
MOTA	1366	CB	LEU A 1	L74 6	2.894	12.838	7.522	1.00 38.73	A
MOTA	1367	CG	LEU A 1	L74 6	2.202	13.329	6.251	1.00 39.18	A
MOTA	1368	CD1	LEU A 1	L74 6	50.826	12.691	6.170	1.00 39.20	A
ATOM	1369	CD2	LEU A 1	L74 6	52.093	14.836	6.245	1.00 40.87	A
MOTA	1370	C	LEU A 1	L74 (4.019	14.662	8.785	1.00 37.43	A
MOTA	1371	0	LEU A 1	L74 (53.630	14.514	9.943	1.00 37.68	A
ATOM	1372	N	LEU A 1	L75 (54.284	15.849	8.255	1.00 35.85	A
ATOM	1373	CA	LEU A 1	L75 (54.098	17.077	9.012	1.00 34.38	A
MOTA	1374	CB	TEU Y 1	L75 (55.400	17.882	9.074	1.00 33.21	A
MOTA	1375	CG	LEU A 1	L75 (66.425	17.502	10.147	1.00 34.82	A
MOTA	1376	CD1	. LEU A I	175 (55.838	17.768	11.526	1.00 34.32	A
MOTA	1377	CD2	LEU A 1	175 (66.819	16.038	10.008	1.00 35.37	A
MOTA	1378	C	LEU A 1	175 (53.020	17.898	8.337	1.00 33.09	A
MOTA	1379	0	LEU A 1	175 (53.080	18.137	7.132	1.00 33.84	A
ATOM	1380	N	LYS A 1	176	62.023	18.312	9.108	1.00 30.14	A
ATOM	1381	CA	LYS A 1	176	60.943	19.119	8.566	1.00 30.03	A
MOTA	1382	CB	LYS A	176	59.598	18.416	8.772	1.00 30.60	A
MOTA	1383	CG	LYS A 1	176	58.463	19.049	8.010	1.00 33.60	A
MOTA	1384	CD	LYS A 1	176	58.742	19.054	6.508	1.00 37.73	A
MOTA	1385	CE	LYS A	176	58.869	17.642	5.960	1.00 37.37	A
MOTA	1386	NZ	LYS A	176	59.075	17.629	4.484	1.00 41.15	A
MOTA	1387	C	LYS A	176	60.976	20.457	9.292	1.00 28.62	A
MOTA	1388	0	LYS A :	176	60.764	20.524	10.501	1.00 27.68	A
MOTA	1389	N	HIS A	177	61.238	21.520	8.539	1.00 28.72	A
ATOM	1390	CA	HIS A	177	61.353	22.868	9.088	1.00 29.54	A
ATOM	1391	СВ	HIS A		62.284	23.691	8.195	1.00 29.51	A
ATOM	1392	CG	HIS A	177	62.485.	25.097	8.663	1.00 30.53	A
MOTA	1393	CD:	HIS A		62.124	26.282	8.114	1.00 31.99	A
ATOM	1394		HIS A		63.117	25.401	9.849	1.00 32.09	A
MOTA	1395		HIS A		63.138	26.713	10.010	1.00 32.65	A
ATOM	1396	NE:	HIS A		62.542	27.271	8.971	1.00 32.04	A
MOTA	1397	С	HIS A		60.059	23.654	9.304	1.00 29.24	A
MOTA	1398	0	A 2IH		59.100	23.519	8.549	1.00 27.66	A
MOTA	1399	N	TRP A		60.062	24.492	10.340	1.00 30.09	A
ATOM	1400	CA			58.926	25.350	10.674	1.00 33.43	A
MOTA	1401	CB	TRP A	178	57.959	24.647	11.632	1.00 28.07	A

ATOM	1402	CG	TRP :	A	178	56.	681	25.422	11.851	1.00	25.25	A
MOTA	1403		TRP :			56.		26.518	12.761		21.68	A
ATOM	1404		TRP .			55.		26.942	12.611		20.86	A
ATOM ATOM	1405 1406		TRP :			57. 55.		27.178 25.239	13.688 11.206		20.72 24.81	A A
ATOM	1405		TRP			54.		26.146	11.657		21.51	A
MOTA	1408		TRP .				598	27.999	13.354		21.11	A
ATOM	1409		TRP				754	28.229	14.428	1.00	21.58	A
MOTA	1410	CH2	TRP	A	178	55.	419	28.627	14.255	1.00	20.94	A
MOTA	1411	C	TRP .				425	26.628	11.348		36.30	A
ATOM	1412	0	TRP				314	26.591	12.195		36.91	A
ATOM	1413	N	GLU .				852	27.761	10.975 11.587		40.65 45.62	A A
ATOM ATOM	1414 1415	CA CB	GLU .				240 481	29.029 29.622	10.899		47.42	A
ATOM	1416	CG	GLU				323	29.868	9.404		52.77	A
ATOM	1417	CD.	GLU				498	30.624	8.806		55.17	A
MOTA	1418	OE1	GLU	A	179	62.	653	30.179	8.987	1.00	57.20	A
MOTA	1419	OE2	GLU	A	179	61.	265	31.663	8.149	1.00	57.21	A
MOTA	1420	C	GLU				074	30.001	11.489		46.47	A
MOTA	1421	0	GLU				322	29.983	10.513		45.49	A
ATOM	1422	И	PRO				898	30.855	12.509		47.97 48.35	A A
ATOM	1423	CD CA	PRO PRO				679 789	31.008 31.810	13.752 12.460		49.45	A
MOTA MOTA	1424 1425	CB	PRO				763	32.372	13.880		49.39	A
ATOM	1426	CG	PRO				214	32.358	14.266		48.65	A
ATOM	1427	C	PRO				014	32.891	11.401	1.00	50.21	A
ATOM	1428	0	PRO	A	180	58.	174	33.041	10.950	1.00	49.95	A
MOTA	1429	OXT	PRO	A	180		030	33.578	11.043		50.90	A
ATOM	1430	CB	SER		3		953	-2.426	7.203		59.72	В
ATOM	1431	OG	SER		3		517	-3.384	6.321		60.71 57.49	B B
ATOM	1432 1433	C O	SER		3 3		.164 .117	-3.822 -4.879	9.277 8.642		57.32	В
ATOM ATOM	1434	N	SER		3		072	-2.418	8.486		59.35	В
ATOM	1435	CA	SER		3		586	-2.517	8.597		58.84	В
ATOM	1436	N	PRO	В	4	67.	855	-3.763	10.585	1.00	55.71	В
ATOM	1437	CD	PRO	В	4	67.	914	-2.580	11.463		54.97	В
MOTA	1438	CA	PRO		4		438	-4.952	11.338		53.72	В
MOTA	1439	CB	PRO		4		457	-4.467	12.787		54.71 54.93	B B
ATOM	1440	CG	PRO PRO		4 4		.095 .069	-3.021 -5.487	12.660 10.918		51.05	В
ATOM ATOM	1441 1442	0	PRO		4		.240	-4.753	10.379		50.96	В
ATOM	1443	N	GLU		5		.843	-6.773	11.165		47.90	В
ATOM	1444	CA	GLU		5	64	.581	-7.410	10.810	1.00	45.24	В
MOTA	1445	CB	GLU	В	5	64	.811	-8.893	10.489		48.23	В
MOTA	1446	CG	GLU		5		.603	-9.656	11.545		54.54	В
ATOM	1447	CD	GLU		5			-11.102	11.140		57.83 59.67	B B
MOTA	1448		GLU GLU		5 5			-11.317 -12.020	10.024 11.941		59.87	В
ATOM ATOM	1449 1450	C	GLU		5		.548	-7.269	11.920		40.85	В
MOTA	1451	ŏ	GLU		5		.876	-7.328	13.105		40.81	В
ATOM	1452	N	ASP		6		.294	-7.083	11.532	1.00	36.03	В
ATOM	1453	CA	ASP	В	6	61	.223	-6.936	12.508		32.11	В
MOTA	1454	CB	ASP		6		.833	-5.460	12.616		29.96	В
ATOM	1455	CG	ASP		6		.933	-5.171	13.798		27.91	В
MOTA	1456		ASP		6		.280 .884	-4.110 -5.982	13.785 14.745		29.62	B B
MOTA MOTA	1457 1458	C	ASP ASP		6 6		.014	-7.766	12.077		29.68	В
ATOM	1459	Ö	ASP				.676	-7.802	10.899		29.14	В
ATOM	1460	N	PHE				.380	-8.438	13.032	1.00	27.77	В
ATOM	1461	CA	PHE	В	7		.193	-9.249	12.765		28.11	В
ATOM	1462	CB	PHE	В	7			-10.704	13.161		29.55	В
ATOM	1463	CG	PHE					-11.385	12.282		31.06	В
MOTA	1464		PHE					-11.766	10.989		29.85 32.21	B B
MOTA MOTA	1465 1466		PHE					-11.603 -12.355	12.730 10.145		33.75	В
MOTA	1467		PHE					-12.190	11.897		34.27	В
ATOM	1468	CZ	PHE					-12.568	10.599	1.00	33.07	В
MOTA	1469	C	PHE				.032	-8.657	13.562		26.58	В
MOTA	1470	0	PHE				.046		14.794		25.72	В
ATOM	1471	N	VAL				.023		12.849		25.17	В
ATOM	1472	CA	VAL				.891		13.493 12.871		23.46	B B
MOTA MOTA	1473 1474	CB CG1	VAL VAL				.670 .573		13.612		21.83	В
ATOM	1475		VAL				.975		12.895		21.30	В
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VAL B ATOM 53.556 -8.255 13.467 1.00 24.08 1476 C 8 В ATOM 1477 VAL B 53.204 -8.912 12.491 1.00 23.46 0 8 ATOM 1478 N TYR B 52.804 -8.127 14.554 1.00 23.26 ATOM TYR B 51.493 -8.747 14.619 1479 CA 9 1.00 23.18 51.510 -9.978 15.520 MOTA 1480 CB TYR B 9 1.00 23.12 В ATOM 1481 CG TYR B 9 50.231 -10.786 15.465 1.00 24.54 ATOM 1482 CD1 TYR B 9 50.158 -11.962 14.722 1.00 26.50 49.000 -12.743 14.716 MOTA 1483 CR1 TYR B 9 1.00 25.08 49.108 ~10.399 16.190 ATOM 1484 CD2 TYR B 9 1.00 22.88 ATOM 1485 CE2 TYR B 9 47.948 -11.165 16.188 1.00 23.91 ATOM 1486 CZ TYR B 9 47.902 -12.342 15.455 1.00 24.87 В 9 1487 46.780 -13.140 15.501 ATTOM OH TYR B 1.00 25.45 В ATOM 1488 C TYR B 50.509 -7.723 15.163 1.00 21.33 В 50.798 -7.028 16.133 ATOM 1489 TYR B 9 1.00 22.92 49.353 -7.622 14.521 48.326 -6.687 14.952 GLN B 10 ATOM 1490 N 1.00 19.98 В ATOM 1491 CA GLN B 10 1.00 19.52 В ATOM 1492 CB GLN B 10 48.171 -5.523 13.962 1.00 19.13 ATOM 1493 CG GLN B 10 49.433 -4.810 13.509 1.00 19.33 CD GLN B 10 49.117 -3.708 12.499 1.00 17.96 MOTA 1494 В ATOM 1495 OE1 GLN B 10 48.336 -2.802 12.783 1.00 18.49 В 1496 NE2 GLN B 10 49.715 -3.790 -11.316 1.00 19.41 В ATOM 46.967 -7.375 15.029 ATOM 1497 C GLN B 10 1.00 19.74 GLN B 10 ATOM 1498 0 46.626 -8.227 14.192 1.00 18.98 В 46.195 -6.996 16.040 ATOM 1499 N PHE B 11 1.00 19.06 R CA PHE B 11 44.842 -7.487 16.182 1.00 16.54 ATOM 1500 ATOM 1501 CB PHE B 11 44.668 -8.454 17.336 1.00 17.48 CG PHE B 11 43.237 -8.847 17.544 1.00 16.17 ATOM 1502 В ATOM 1503 CD1 PHE B 11 42.570 -9.604 16.582 1.00 17.49 -8.406 18.656 CD2 PHE B 11 42.536 1.00 14.41 ATOM 1504 В ATOM 1505 CE1 PHE B 11 41.219 -9.913 16.725 1.00 18.03 CE2 PHE B 11 41.191 -8.708 18.814 1.00 16.34 ATOM 1506 MOTA 1507 CZ PHE B 11 40.528 -9.463 17.845 1.00 17.60 В PHE B 11 43.984 -6.271 16.450 1.00 18.14 MOTA 1508 С PHE B 11 44.241 -5.506 17.386 1.00 15.63 В MOTA 1509 0 42.961 -6.094 15.625 1.00 17.33 LYS B 12 MOTA 1510 N В MOTA 1511 CA LYS B 12 42.082 -4.958 15.770 1.00 17.63 В MOTA 1512 CB LYS B 12 42.188 -4.067 14.536 1.00 18.71 В 43.599 -3.642 14.192 1.00 15.90 ATOM 1513 CG LYS B 12 43.602 -2.909 12.871 44.946 -2.297 12.570 CD LYS B 12 1.00 17.33 В MOTA 1514 MOTA 1515 CE LYS B 12 1.00 18.72 В 1516 NZ LYS B 12 44.838 -1.450 11.340 1.00 20.93 MOTA MOTA C LYS B 12 40.632 -5.387 15.968 1.00 18.92 1517 40.041 -6.050 15.109 1.00 17.25 MOTA 1518 0 LYS B 12 В N MOTA 1519 GLY B 13 40.076 -5.002 17.114 1.00 17.59 B GLY B 13 38.701 -5.322 17.430 1.00 19.88 MOTA 1520 CA В 37.874 -4.113 17.064 GLY B 13 1.00 20.12 MOTA 1521 С 37.515 -3.309 17.923 GLY B 13 MOTA 1522 0 1.00 21.08 В MOTA 1523 N MET B 14 37.561 -4.000 15.779 1.00 20.42 В 36.817 -2.866 CA MET B 14 15.262 1.00 22.96 ATOM 1524 MET B 14 37.334 -2.554 13.866 1.00 23.02 В **ATOM** 1525 CB 38.846 -2.485 MET B 14 13.820 1.00 23.58 В ATOM 1526 CG ATOM 1527 SD MET B 14 39.449 -2.095 12.191 1.00 26.23 В MET B 14 39.260 -0.318 12.182 1.00 25.78 ATOM 1528 CE В 35.295 -2.997 ATOM 1529 C MET B 14 15.242 1.00 23.12 ATOM MET B 14 34.751 -4.089 15.081 1.00 24.36 В 1530 0 34.628 -1.860 ATOM 1531 N CYS B 15 15.427 1.00 24.04 В 33.173 -1.768 15.433 1.00 24.91 ATOM 1532 CA CYS B 15 CYS B 15 CYS B 15 MOTA 1533 C 32.808 -0.587 14.547 1.00 25.49 33.369 0.504 14.700 1.00 23.97 MOTA 1534 0 В 16.847 1.00 26.02 ATOM 1535 CB CYS B 15 32.630 -1.489 В ATOM 1536 SG CYS B 15 32.691 -2.831 18.084 1.00 33.69 В TYR B 16 31.871 -0.805 13.630 1.00 25.87 ATOM 1537 N 31.413 12.724 1.00 25.59 ATOM CA TYR B 16 0.244 1538 ATOM 1539 CB TYR B 16 31.539 -0.223 11.274 1.00 24.73 ATOM 1540 CG TYR B 16 32.958 -0.575 10.879 1.00 26.05 MOTA 33.523 -1.795 11.239 1.00 22.96 1541 CD1 TYR B 16 34.843 -2.102 10.904 1.00 25.81 MOTA 1542 CE1 TYR B 16 MOTA 1543 CD2 TYR B 16 33.748 0.334 10.171 1.00 25.30 MOTA 1544 35.066 0.041 9.835 1.00 25.12 CE2 TYR B 16 ATOM 1545 CZ TYR B 16 35.607 -1.176 10.202 1.00 26.66 MOTA 36.908 9.868 1.00 29.22 1546 TYR B 16 -1.463 OH ATOM 1547 C TYR B 16 29.960 0.575 13.045 1.00 26.48 ATOM 29.113 -0.315 1548 0 TYR B 16 13.091 1.00 26.41 ATOM 1549 N PHE B 17 29.684 1.859 13.266 1.00 27.76

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MOTA	1550	CA	PHE	В	17	28.346	2.338	13.613	1.00 29.09	В
ATOM	1551	CB	PHE 1	В	17	28.382	3.047	14.967	1.00 28.08	В
MOTA	1552	CG	PHE	В	17	28.885	2.194	16.091	1.00 28.21	В
ATOM	1553	CD1	PHE !	В	17	28.056	1.253	16.693	1.00 27.20	В
MOTA	1554	CD2	PHE :	В	17	30.188	2.340	16.558	1.00 26.60	В
ATOM	1555	CE1	PHE	В	17	28.519	0.470	17.752	1.00 28.13	В
MOTA	1556		PHE		17	30.662	1.565	17.610	1.00 25.62	В
			PHE			29.828	0.629	18.210	1.00 26.17	В
ATOM	1557	.cz			17					
MOTA	1558	C	PHE		17	27.772	3.318	12.592	1.00 30.71	В
MOTA	1559	0	PHE	В	17	28.452	4.239	12.155	1.00 31.05	В
ATOM	1560	N	THR	В	18	26.506	3.125	12.237	1.00 33.51	В
MOTA	1561	CA	THR	В	18	25.831	4.005	11.291	1.00 36.95	В
MOTA	1562	CB	THR	В	18	25.797	3.395	9.875	1.00 37.23	В
ATOM	1563		THR	В	18	27.133	3.105	9.447	1.00 40.77	В
ATOM	1564		THR		18	25.171	4.369	8.891	1.00 38.43	В
	1565	C	THR		18	24.398	4.273	11.753	1.00 38.56	В
ATOM								12.131	1.00 38.36	В
ATOM	1566	0	THR		18	23.671	3.351			В
ATOM	1567	N	asn		19	24.007	5.544	11.726	1.00 39.80	
MOTA	1568	CA	asn	В	19	22.668	5.961	12.132	1.00 41.35	В
ATOM	1569	CB	ASN	В	19	21.638	5.465	11.110	1.00 41.21	В
MOTA	1570	CG	asn	В	19	20.311	6.190	11.223	1.00 42.85	В
MOTA	1571	OD1	ASN	В	19	20.271	7.378	11.548	1.00 42.24	В
ATOM	1572		ASN		19	19.219	5.485	10.937	1.00 42.57	В
ATOM	1573	C	ASN		19	22.352	5.416	13.521	1.00 42.37	В
					19	21.540	4.503	13.673	1.00 43.36	В
MOTA	1574	.0	ASN						1.00 42.56	В
MOTA	1575	N	GLY		20	22.997	5.989	14.533		
MOTA	1576	CA	GLY		20	22.790	5.535	15.894	1.00 43.89	В
MOTA	1577	С	GLY	В	20	23.293	4.110	16.031	1.00 45.10	В
MOTA	1578	0	GLY	В	20	24.421	3.807	15.646	1.00 44.28	В
ATOM	1579	N	THR	В	21	22.458	3.232	16.575	1.00 46.37	В
ATOM	1580	CA	THR	В	21	22.824	1.832	16.738	1.00 47.42	В
ATOM	1581	СВ	THR		21	22.667	1.373	18.199	1.00 48.57	В
ATOM	1582		THR		21	21.438	1.885	18.731	1.00 49.14	В
ATOM	1583		THR		21	23.843	1.856	19.043	1.00 47.59	В
							0.947	15.846	1.00 48.74	В
MOTA	1584	C	THR		21	21.958				В
MOTA	1585	0	THR		21	21.925	-0.276	16.016	1.00 48.04	
ATOM	1586	N	GLU	₿	22	21.253	1.570	14.902	1.00 48.57	В
MOTA	1587	CA	GLU	В	22	20.405	0.822	13.979	1.00 48.90	В
ATOM	1588	CB	GLŪ	В	22	19.741	1.745	12.957	1.00 52.60	В
ATOM	1589	CG	GLU	В	22	18.669	2.667	13.493	1.00 58.06	В
ATOM	1590	œ	GLU		22	17.862	3.297	12.368	1.00 62.27	В
ATOM	1591		GLU		22	17.027	4.185	12.648	1.00 63.99	В
			GLU		22	18.065	2.894	11.199	1.00 64.70	В
ATOM	1592				22	21.285	-0.156	13.229	1.00 46.38	В
ATOM	1593	C	GLU				-1.356	13.209	1.00 45.52	В
ATOM	1594	0	GLU		22	21.029				В
MOTA	1595	N	ARG		23	22.324	0.379	12.601	1.00 45.42	
MOTA	1596	CA	ARG		23	23.260	-0.438	11.844	1.00 44.59	В
MOTA	1597	CB	ARG	В	23	23.423	0.127	10.422	1.00 45.69	В
MOTA	1598	CG	ARG	В	23	22.169	-0.062	9.554	1.00 49.95	В
MOTA	1599	CD	ARG	В	23	22.406	0.237	8.074	1.00 53.34	В
ATOM	1600	NE	ARG		23	22,153	1.632	7.708	1.00 55.57	В
ATOM	1601	CZ	ARG	B	23	20.949	2.200	7.700	1.00 57.20	В
ATOM	1602		ARG		23	19.878	1.495	8.042	1.00 58.09	В
			ARG		23	20.813	3.471	7.340	1.00 56.82	В
ATOM	1603					24.606	-0.534	12.567	1.00 40.56	В
MOTA	1604	C	ARG		23				1.00 41.15	В
MOTA	1605	0	ARG		23	25.306	0.459	12.748		
ATOM	1606	N	VAL		24	24.944	-1.743	12.995	1.00 38.17	В
MOTA	1607	CA	VAL	В	24	26.191	-1.996	13.708	1.00 34.88	В
MOTA	1608	CB	VAL	В	24	25.931	-2.314	15.200	1.00 34.41	В
MOTA	1609	CG1	L VAL	В	24	27.251	-2.526	15.918	1.00 35.28	В
MOTA	1610		VAL		24	25.146	-1.190	15.852	1.00 34.70	В
MOTA	1611	C	VAL		24	26.909	-3.194	13.100	1.00 32.34	В
ATOM	1612	õ	VAL		24	26.287	-4.214	12.812	1.00 33.23	В
						28.217	-3.076	12.898	1.00 30.18	В
ATOM	1613	N	ARG		25	28.970			1.00 26.97	В
ATOM	1614	CA	ARG		25		-4.194	12.354		В
ATOM	1615	CB	ARG		25	29.225	-4.022	10.852	1.00 27.67	
MOTA	1616	CG	ARG		25	29.400	-5.362	10.170	1.00 29.58	В
MOTA	1617	ÇD	ARG	В	25	30.406	-5.363	9.052	1.00 31.26	В
ATOM	1618	NE	ARG	В	25	30.058	-4.454	7.974	1.00 33.12	В
ATOM	1619		ARG		25	30.415	-4.631	6.705	1.00 32.27	В
ATOM	1620		1 ARG		25	31.124	-5.695	6.346	1.00 31.13	В
ATOM	1621		2 ARG		25	30.087	-3.726	5.799	1.00 30.62	В
ATOM			ARG		25	30.305	-4.402	13.065	1.00 24.10	В
	1622					31.095	-3.477	13.225	1.00 22.56	В
MOTA	1623	0	ARG	. 5	25	51.055	-3.4//	20.00	2.00 22.00	_

3.0004	7.004	NT.	LEU	-	26	30.551	-5.630	33 405	1.00 22.65	В
ATOM	1624	N			26			13.495		
ATOM	1625	CA	LEU		26	31.801	-5.942	14.163	1.00 22.38	В
MOTA	1626	CB	ΓEΩ		26	31.558	-6.888	15.345	1.00 20.25	В
ATOM	1627	CG	ΓEΩ		26	32.795	-7.389	16.100	1.00 19.86	В
MOTA	1628	CD1	LEU	В	26	32.452	-7.613	17.568	1.00 22.49	В
ATOM	1629	CD2	LEU	В	26	33.304	-8.665	15.464	1.00 18.43	В
MOTA	1630	С	LEU	В	26	32.726	-6.591	13.150	1.00 21.50	В
ATOM	1631	ō	LEU		26	32.289	-7.402	12.342	1.00 22.83	В
									1.00 21.29	В
ATOM	1632	N	VAL		27	33.998	-6.208	13.177		
ATOM	1633	CA	VAL		27	34.984	-6.780	12.270	1.00 20.66	В
ATOM	1634	CB	VAL		27	35.178	-5.911	11.004	1.00 20.59	В
ATOM	1635	CG1	VAL	В	27	36.169	-6.576	10.069	1.00 19.45	В
ATOM	1636	CG2	VAL	В	27	33.849	-5.696	10.297	1.00 22.37	В
ATOM	1637	C	VAL	В	27	36.330	-6.885	12.988	1.00 22.39	В
ATOM	1638	ō	VAL		27	37.046	-5.889	13.135	1.00 22.63	В
									1.00 21.32	
MOTA	1639	N	SER		28	36.673	-8.083	13.450		В
ATOM	1640	CA	SER		28	37.947	-8.259	14.130	1.00 21.51	В
ATOM	1641	CB	SER	В	28	37.831	-9.284	15.275	1.00 19.72	В
MOTA	1642	OG	SER	В	28	37.542	-10.581	14.819	1.00 24.33	В
ATOM	1643	С	SER	В	28	38.954	-8.693	13.074	1.00 21.25	В
ATOM	1644	ō	SER		28	38.661	-9.537	12.229	1.00 19.44	В
		N	ARG		29	40.137	-8.089	13.106	1.00 20.61	В
MOTA	1645									
ATOM	1646	CA	ARG		29	41.158	-8.402	12.115	1.00 19.66	В
MOTA	1647	CB	ARG		29	41.418	-7.169	11.230	1.00 19.91	В
MOTA	1648	CG	ARG	В	29	40.178	-6.407	10.754	1.00 16.79	В
ATOM	1649	CD	ARG	В	29	40.608	-5.121	10.031	1.00 18.10	В
MOTA	1650	NE	ARG	В	29	39.487	-4.318	9.553	1.00 19.38	В
MOTA	1651	CZ	ARG		29	38.738	-4.619	8.497	1.00 20.62	В
			ARG		29	38.983	-5.714	7.789	1.00 19.50	В
MOTA	1652									
MOTA	1653	NH2			29	37.736	-3.822	8.149	1.00 21.90	В
MOTA	1654	C	ARG	В	29	42.482	-8.833	12.738	1.00 18.57	В
MOTA	1655	0	ARG	В	29	43.024	-8.121	13.584	1.00 19.40	В
ATOM	1656	N	SER	В	30	42.991	-9.995	12.326	1.00 18.99	В
ATOM	1657	CA	SER	В	30	44.284	-10.501	12.797	1.00 21.66	В
ATOM	1658	CB	SER		30		-12.015	13.023	1.00 22.77	В
		OG	SER		30		-12.352	14.106	1.00 26.81	В
MOTA	1659									В
ATOM	1660	C	SER		30		-10.163	11.673	1.00 23.37	
MOTA	1661	0	SER		30		-10.553	10.522	1.00 21.31	В
MOTA	1662	N	ILE	В	31	46.338	-9.450	12.009	1.00 24.76	В
ATOM	1663	CA	ILE	В	31	47.298	-8.998	10.999	1.00 24.33	В
MOTA	1664	CB	ILE	В	31	47.341	-7.440	10.958	1.00 25.20	В
ATOM	1665		ILE		31	47.982	-6.964	9.672	1.00 23.24	В
			ILE		31	45.934	-6.857	11.106	1.00 26.96	В
ATOM	1666									В
MOTA	1667		ILE		31	45.032	-7.136	9.947	1.00 31.25	
ATOM	1668	С	ILE		31	48.741	-9.460	11.187	1.00 23.98	В
ATOM	1669	0	IFE	В	31	49.298	-9.318	12.272	1.00 22.29	В
ATOM	1670	N	TYR	В	32	49.345	-9.993	10.123	1.00 25.50	В
ATOM	1671	CA	TYR	В	32	50.750	-10.405	10.162	1.00 26.21	В
ATOM	1672	CB	TYR		32	50.965	-11.764	9.492	1.00 28.46	В
			TYR				-12.224	9.544	1.00 31.10	В
ATOM	1673	CG			32					
MOTA	1674		TYR		32		-12.412	10.765	1.00 32.47	В
ATOM	1675		TYR		32		-12.780	10.827	1.00 34.69	В
ATOM	1676	CD2	TYR	В	32		-12.424	8.375	1.00 33.60	В
ATOM	1677	CE2	TYR	В	32	54.484	-12.795	8.422	1.00 34.50	В
ATOM	1678	\mathbf{cz}	TYR	В	32	55.103	-12.965	9.654	1.00 35.65	В
MOTA	1679	OH	TYR		32	56.438	-13.281	9.717	1.00 37.73	В
ATOM	1680	C	TYR		32	51.478	-9.307	9.384	1.00 25.67	В
						51.273			1.00 24.75	В
MOTA	1681	0	TYR		32		-9.140	8.174		
MOTA	1682	N	ASN		33	52.319	-8.559	10.094	1.00 25.63	В
MOTA	1683	ÇA	asn	В	33	53.036	-7.416	9.526	1.00 24.95	В
MOTA	1684	СВ	asn	В	33	53.955	-7.848	8.379	1.00 23.75	В
MOTA	1685	CG	ASN	В	33	55.171	-8.615	8.878	1.00 24.11	В
MOTA	1686		ASN		33	55.803	-8.223	9.861	1.00 25.42	В
ATOM			ASN		33	55.506	-9.708	8.204	1.00 25.18	В
	1687					51.990		9.070	1.00 25.11	В
ATOM	1688	C	ASN		33					
ATOM	1689	0	asn		33	51.491		9.893	1.00 26.06	В
MOTA	1690	'n	ARG		34	51.652		7.786	1.00 25.75	В
MOTA	1691	CA	ARG	В	34	50.631	-5.449	7.296	1.00 27.64	В
ATOM	1692	CB	ARG	В	34	51.244	-4.362	6.408	1.00 27.74	В
ATOM	1693	CG	ARG		34	51.972		7.158	1.00 29.94	В
MOTA	1694	CD	ARG		34	51.664		6.541	1.00 32.95	В
						51.897		5.101	1.00 35.17	В
MOTA	1695	NB	ARC		34					
MOTA	1696	CZ	ARG		34	51.392		4.267	1.00 37.51	В
MOTA	1697	NH:	LARC	3 B	34	50.622	0.003	4.729	1.00 39.45	В

ATOM	1698	NH2	ARG	В	34	51.642	-1.058	2.967	1.00 36.90	В
ATOM	1699	C	ARG		34	49.587	-6.218	6.498	1.00 26.48	В
MOTA	1700	0	ARG	В	34	48.740	-5.639	5.825	1.00 27.17	В
MOTA	1701	N	GLU	В	35	49.647	-7.534	6.602	1.00 25.66	В
MOTA	1702	CA	GLU		35	48.746	-8.394	5.867	1.00 26.99	В
MOTA	1703	CB	GLU		35	49.570	-9.483	5.175	1.00 31.53	В
ATOM	1704	CG	GT 1		35		-10.396	4.235	1.00 36.29	В
ATOM	1705	CD	GLU		35		-11.530	3.731	1.00 40.61	В
ATOM	1706		GLU		35		-11.240	3.276	1.00 45.20	В
ATOM	1707		GLU		35		-12.705	3.791	1.00 41.13	В
MOTA MOTA	1708 1709	С 0	GLU		35 35	47.699 48.028	-9.031 -9.807	6.764 7.663	1.00 25.09 1.00 23.31	B B
MOTA	1710	N	GLU		36	46.439	-8.689	6.522	1.00 24.53	В
ATOM	1711	CA	GLU		36	45.332	-9.263	7.275	1.00 25.73	В
ATOM	1712	СВ	GLU		36	44.023	-8.519	6.958	1.00 26.62	В
ATOM	1713	CG	GLU		36	42.783	-9.095	7.636	1.00 28.26	В
MOTA	1714	СD	GLU	В	36	41.545	-8.232	7.442	1.00 31.08	В
ATOM	1715	OB1	GLU	В	36	41.420	-7.590	6.377	1.00 32.56	В
ATOM	1716	OE2	GLU	В	36	40.685	-8.206	8.349	1.00 32.83	В
ATOM	1717	C	GLU		36	45.238	-10.717	6.822	1.00 24.67	В
ATOM	1718	0	GLU		36		-10.992	5.626	1.00 23.91	В
MOTA	1719	N	ILE		37		-11.647	7.771	1.00 26.11	В
ATOM	1720	CA	ILE		37		-13.067	7.433	1.00 27.80	В
ATOM	1721	CB	ILE		37		-13.822	8.013 7.516	1.00 27.27 1.00 27.41	B B
MOTA MOTA	1722 1723		ILE		37 37		-13.174 -13.767	9.537	1.00 27.41	В
ATOM	1724		ILE		37		-14.509	10.175	1.00 30.27	В
ATOM	1725	C	ILE		37		-13.750	7.879	1.00 27.86	В
ATOM	1726	ō	ILE		37		-14.674	7.221	1.00 28.29	В
ATOM	1727	N	VAL		38		-13.296	8.989	1.00 28.78	В
MOTA	1728	CA	VAL	В	38	42.097	-13.870	9.487	1.00 29.29	В
MOTA	1729	CB	VAL	В	38	42.294	-14.751	10.741	1.00 30.18	В
ATOM	1730		VAL		38	40.983	-15.452	11.071	1.00 33.17	В
ATOM	1731		VAL		38		-15.764	10.520	1.00 31.09	В
MOTA	1732	C	VAL		38		-12.745	9.882	1.00 28.75	В
MOTA	1733	0	VAL		38		-11.758	10.480	1.00 29.70	В
ATOM	1734	N	ARG		39		-12.911	9.581	1.00 27.05 1.00 25.46	B B
ATOM	1735	CA CB	ARG ARG		39 39		-11.890 -11.064	9.892 8.632	1.00 27.23	В
ATOM ATOM	1736 1737	CG	ARG		39		-10.011	8.765	1.00 30.84	В
ATOM	1738	CD	ARG		39	37.111	-9.476		1.00 29.34	В
ATOM	1739	NE	ARG		39	38,218	-8.861	6.673	1.00 30.83	В
ATOM	1740	CZ	ARG		39	38.116	-8.328	5.459	1.00 31.23	В
ATOM	1741		ARG	В	39	36.951	-8.333	4.823	1.00 31.08	В
MOTA	1742	NH2	ARG	В	39	39.178	-7.779	4.883	1.00 30.81	В
ATOM	1743	C	ARG	В	39	37.573	-12.476	10.381	1.00 25.41	В
MOTA	1744	0	ARG		39		-13.587	9.996	1.00 25.06	В
MOTA	1745	N	PHE		40		-11.742	11.252	1.00 23.72	В
ATOM	1746	CA	PHE		40		-12.164	11.696	1.00 24.04	В
MOTA	1747	CB	PHE		40 40		-12.554 -13.036	13.171 13.573	1.00 22.69 1.00 20.75	B B
ATOM ATOM	1748 1749		PHE		40		-14.370	13.413	1.00 20.73	В
ATOM	1750		PHE		40		-12.135	14.003	1.00 21.00	В
ATOM	1751		PHE		40		-14.800	13.670	1.00 20.86	В
ATOM	1752		PHE		40		-12.553	14.261	1.00 19.95	В
ATOM	1753	CZ	PHE		40	31.517	-13.890	14.092	1.00 19.78	В
MOTA	1754	C	PHE	В	40	34.662	-10.969	11.474	1.00 24.27	В
MOTA	1755	0	PHE		40	34.755	-9.970	12.183	1.00 22.94	В
MOTA	1756	N	ASP		41		-11.088	10.471	1.00 24.75	В
ATOM	1757	CA	ASP		41		-10.040	10.101	1.00 24.98	В
MOTA	1758	CB	ASP		41 41	32.863 32.162	-9.881 -8.626	8.578 8.116	1.00 25.64 1.00 27.70	B B
MOTA MOTA	1759 1760	CG	ASP ASP		41	31.163	-8.227	8.749	1.00 26.21	В
MOTA	1761		ASP		41	32.607		7.102	1.00 30.42	В
ATOM	1762	C	ASP		41		-10.497	10.560	1.00 24.50	В
MOTA	1763	0	ASP		41		-11.558	10.151	1.00 24.95	В
ATOM	1764	N	SER		42	30.822		11.404	1.00 24.16	В
MOTA	1765	CA	SER	В	42	29.501	-10.096	11.882	1.00 26.13	В
ATOM	1766	CB	SER		42	29.013		12.972	1.00 24.53	В
MOTA	1767	OG	SER		42	28.932		12.497	1.00 23.39	В
ATOM	1768	C	SER		42		-10.149	10.729	1.00 27.68	В
MOTA	1769	0	SER		42 43		-10.833	10.818	1.00 27.31 1.00 28.17	B B
MOTA MOTA	1770 1771	N CA	ASP ASP		43 43	28.789 27.924		9.654 8.477	1.00 29.40	В
WT ON	1//1	LA.	ALC C			-1.744	- 2.413	3.411		

ATOM	1772	СВ	ASP	В	43	28.332 -8.298 7.508 1.00 29.57	В
MOTA	1773	CG	ASP	В	43	27.587 -7.006 7.766 1.00 32.71	В
MOTA	1774	OD1	ASP	В	43	26.999 -6.868 8.862 1.00 33.94	В
MOTA	1775		asp		43	27.593 -6.120 6.881 1.00 33.98	В
ATOM	1776	C	ASP		43	28.036 -10.762 7.782 1.00 29.46	В
MOTA	1777	0	ASP		43	27.162 -11.150	B B
ATOM ATOM	1778 1779	n Ca	VAL VAL		44	29.365 -12.780 7.486 1.00 27.16	В
MOTA	1780	CB	VAL		44	30.846 -12.939 7.075 1.00 27.32	В
ATOM	1781		VAL		44	31.083 -14.323 6.488 1.00 24.09	В
ATOM	1782		VAL		44	31.218 -11.857 6.073 1.00 24.66	В
MOTA	1783	C	VAL	В	44	28.990 -13.867 8.490 1.00 28.43	В
MOTA	1784	0	VAL	В	44	28.558 -14.948 8.108 1.00 29.45	В
ATOM	1785	N	GLY		45	29.177 -13.590 9.774 1.00 28.05	В
ATOM	1786	CA	GLY		45	28.794 -14.561 10.780 1.00 28.67	В
MOTA	1787	C	GLY		45	29.758 -15.679 11.125 1.00 28.25 29.458 -16.486 12.002 1.00 29.67	B B
MOTA	1788	0	GLY GLU		45 46	29.458 -16.486 12.002 1.00 29.67 30.895 -15.755 10.443 1.00 27.03	В
MOTA MOTA	1789 1790	N CA	GTO		46	31.873 -16.787 10.757 1.00 29.26	В
ATOM	1791	CB	GLU		46	31.571 -18.087 10.000 1.00 32.16	В
ATOM	1792	CG	GLU		46	32.039 -18.121 8.554 1.00 37.36	В
ATOM	1793	CD	GLU	В	46	31.752 -19.458 7.885 1.00 41.59	В
MOTA	1794	OE1	elu	В	46	32.163 -20.505 8.433 1.00 43.30	В
MOTA	1795	OR2	GLU		46	31.116 -19.463 6.810 1.00 43.54	В
ATOM	1796	C	GLU		46	33.272 -16.295 10.413 1.00 29.29	В
ATOM	1797	0	GLU		46	33.432 -15.288 9.722 1.00 30.45	B B
ATOM	1798	N	PHE		47	34.281 -17.005 10.904 1.00 28.00 35.670 -16.650 10.651 1.00 28.10	В
ATOM ATOM	1799 1800	CA CB	PHE		47 47	36.594 -17.445 11.566 1.00 28.74	В
ATOM	1801	CG	PHE		47	36.487 -17.067 13.016 1.00 30.23	В
ATOM	1802		PHE		47	37.248 -16.023 13.535 1.00 28.96	В
ATOM	1803		PHE		47	35.636 -17.768 13.870 1.00 30.80	В
ATOM	1804	CE1	PHE	В	47	37.166 -15.683 14.888 1.00 31.59	В
ATOM	1805	CE2	PHE		47	35.544 -17.435 15.229 1.00 31.97	B
ATOM	1806	CZ	PHE		47	36.311 -16.392 15.737 1.00 30.36	В
ATOM	1807	C	PHE		47	36.034 -16.948 9.211 1.00 28.71	B
MOTA	1808	0	PHE		47	35.576 -17.937 8.640 1.00 28.03 36.872 -16.091 8.637 1.00 27.96	В
ATOM ATOM	1809 1810	n Ca	ARG		48 48	37.327 -16.242 7.261 1.00 26.41	В
ATOM	1811	CB	ARG		48	36.513 -15.341 6.326 1.00 26.57	В
ATOM	1812	CG	ARG		48	35.068 -15.755 6.108 1.00 26.19	В
MOTA	1813	CD	ARG	В	48	34.971 -17.079 5.352 1.00 24.98	В
ATOM	1814	NE	ARG	B	48	33.579 -17.465 5.146 1.00 26.01	В
ATOM	1815	CZ	ARG		48	32.755 -16.867 4.294 1.00 26.84	В
ATOM	1816		ARG		48	33.181 -15.857 3.554 1.00 26.92	В
ATOM	1817		ARG		48	31.492 -17.260 4.204 1.00 30.22 38.799 -15.861 7.140 1.00 26.95	B
MOTA	1818	C	ARG ARG		48 48	38.799 -15.861 7.140 1.00 26.95 39.255 -14.878 7.737 1.00 24.36	В
MOTA MOTA	1819 1820	N	ALA		49	39.542 -16.647 6.373 1.00 24.93	В
ATOM	1821	CA	ALA		49	40.943 -16.349 6.143 1.00 26.58	В
ATOM	1822	СВ	ALA		49	41.709 -17.619 5.792 1.00 27.05	В
ATOM	1823	C	ALA	В	49	40.927 -15.397 4.956 1.00 26.47	В
MOTA	1824	0	ALA		49	40.210 -15.635 3.983 1.00 26.12	В
MOTA	1825	N	VAL		50	41.674 -14.302 5.044 1.00 27.06	В
MOTA	1826	CA	VAL		50	41.720 -13.357 3.936 1.00 26.50 41.790 -11.876 4.439 1.00 27.14	B
MOTA	1827	CB	VAL VAL		50 50	41.790 -11.876	В
ATOM ATOM	1828 1829		VAL		50	42.628 -11.020 3.501 1.00 27.33	В
MOTA	1830	C	VAL		50	42.891 -13.742 3.037 1.00 26.58	В
MOTA	1831	ō	VAL		50	42.914 -13.390 1.860 1.00 27.84	В
MOTA	1832	N	THR	В	51	43.842 -14.489 3.598 1.00 26.61	В
MOTA	1833	CA	THR	В	51	44.992 -15.011 2.846 1.00 28.59	В
MOTA	1834	CB	THR		51	46.295 -14.193 3.056 1.00 28.25	В
MOTA	1835		THR		51	46.828 -14.464 4.356 1.00 28.56	В
ATOM	1836		THR		51 51	46.033 -12.699 2.899 1.00 27.40 45.256 -16.435 3.344 1.00 29.29	B B
ATOM	1837	C	THR		51 51	45.256 -16.435 3.344 1.00 29.29 44.787 -16.818 4.418 1.00 30.16	В
MOTA MOTA	1838 1839	Ŋ	LEU		52	46.005 -17.217 2.575 1.00 30.64	В
ATOM	1840	CA	LEU		52	46.309 -18.596 2.959 1.00 31.32	В
ATOM	1841	СВ	LEU		52	47.277 -19.237 1.963 1.00 32.19	В
ATOM	1842	CG	LEU		52	46.706 -19.724 0.624 1.00 36.90	В
MOTA	1843		LLEU		52	47.836 -20.306 -0.216 1.00 35.68	В
MOTA	1844		2 LEU		52	45.620 -20.775 0.861 1.00 35.34	В
ATOM	1845	C	LEU	В	52	46.892 -18.724 4.359 1.00 31.57	В

ATOM	1846	0	LEU B	52	46.570 -19.656 5.097 1.00 31.50	В
ATOM	1847	N	LEU B	53	47.753 -17.786 4.723 1.00 31.09	В
MOTA	1848	CA	LEU B	53	48.388 -17.815 6.029 1.00 30.93	В
ATOM	1849	CB	LEU B		49.160 -16.511 6.246 1.00 31.99	В
ATOM ATOM	1850 1851	CG	LEU B		50.338 -16.532	B B
ATOM	1852		PEO B		50.975 -15.148 7.284 1.00 34.96	В
ATOM	1853	C	LEU B		47.377 -18.017 7.160 1.00 29.90	В
ATOM	1854	ō	LEU B		47.663 -18.709 8.138 1.00 30.68	В
ATOM	1855	N	GLY B		46.192 -17.430 7.015 1.00 28.63	В
MOTA	1856	CA	GLY B	54	45.181 -17.537 8.057 1.00 29.75	В
ATOM	1857	C	GLY B	54	44.140 -18.635 7.901 1.00 30.44	В
ATOM	1858	0	GLY B		43.146 -18.664 8.630 1.00 28.02	В
MOTA	1859	N	TEA B		44.364 -19.547 6.964 1.00 30.54	В
MOTA	1860	CA	TEG B		43.417 -20.630 6.732 1.00 32.59	B B
ATOM	1861	CB	LEU B		43.765 -21.344	В
ATOM ATOM	1862 1863	CG	LEU B		42.776 -22.383	В
ATOM	1864		LEU B		43.173 -22.766 3.467 1.00 39.03	В
ATOM	1865	c	LEU B		43.330 -21.631 7.892 1.00 32.20	В
ATOM	1866	ō	LEU B		42.235 -22.026 8.291 1.00 33.32	В
ATOM	1867	N	PRO B	56	44.478 -22.058 8.447 1.00 31.03	В
ATOM	1868	CD	PRO B	56	45.862 -21.802 8.009 1.00 30.17	В
ATOM	1869	CA	PRO B		44.451 -23.013 9.561 1.00 30.23	В
ATOM	1870	CB	PRO B		45.925 -23.148 9.931 1.00 30.27	В
MOTA	1871	CG	PRO B		46.609 -22.967 8.610 1.00 28.92	В
MOTA	1872	C	PRO E		43.613 -22.525 10.740 1.00 31.42 42.730 -23.237 11.222 1.00 33.17	B B
MOTA	1873 1874	0	PRO B		42.730 -23.237 11.222 1.00 33.17 43.893 -21.305 11.196 1.00 30.04	В
MOTA MOTA	1875	N CA	ALA E		43.181 -20.719 12.322 1.00 28.60	В
ATOM	1876	СВ	ALA E		43.818 -19.389 12.697 1.00 26.81	В
ATOM	1877	c	ALA E		41.695 -20.528 12.021 1.00 29.08	В
ATOM	1878	ō	ALA E		40.847 -20.737 12.887 1.00 28.22	В
ATOM	1879	N	ALA E	3 58	41.385 -20.135 10.791 1.00 28.84	В
MOTA	1880	CA	ALA E	3 58	40.002 -19.922 10.386 1.00 31.06	В
MOTA	1881	CB	ALA E		39.955 -19.426 8.947 1.00 29.79	В
MOTA	1882	C	ALA E		39.169 -21.199 10.529 1.00 32.38	В
MOTA	1883	0	ALA E		38.113 -21.197 11.170 1.00 31.57	B B
ATOM	1884	N	GLU E		39.647 -22.285	В
MOTA	1885	CA	GLU E		38.949 -23.565	В
ATOM ATOM	1886 1887	CB	GLU I		39.619 -24.457 7.696 1.00 39.73	В
MOTA	1888	CD	GLU F		40.327 -25.583 6.957 1.00 43.58	В
ATOM	1889		GLU I		41.561 -25.715 7.119 1.00 44.52	В
MOTA	1890	OE2	GLU I	3 59	39.648 -26.337 6.222 1.00 44.30	В
MOTA	1891	С	GLU I	B 59	38.771 -24.063 11.425 1.00 33.56	В
MOTA	1892	0	GPA 1		37.708 -24.570 11.790 1.00 34.40	В
MOTA	1893	N	TYR I		39.815 -23.923 12.233 1.00 31.99	В
MOTA	1894	CA	TYR 1		39.754 -24.369 13.611 1.00 31.01 41.112 -24.202 14.292 1.00 31.13	B B
MOTA	1895	CB	TYR I		41.112 -24.202 14.292 1.00 31.13 41.051 -24.548 15.750 1.00 30.99	В
MOTA MOTA	1896	CG	TYR I TYR I		40.919 -25.871 16.162 1.00 32.55	В
ATOM	1897 1898		TYR		40.770 -26.192 17.508 1.00 35.39	В
ATOM	1899		TYR		41.039 -23.550 16.716 1.00 32.67	В
ATOM	1900		TYR		40.890 -23.853 18.064 1.00 35.14	В
ATOM	1901	CZ	TYR		40.756 -25.177 18.455 1.00 36.91	В
ATOM	1902	OH	TYR I	B 60	40.606 -25.483 19.791 1.00 40.06	В
ATOM	1903	C	TYR :	B 60	38.695 -23.631 14.426 1.00 31.72	В
MOTA	1904	0	TYR :		37.840 -24.258 15.050 1.00 31.72	В
MOTA	1905	N	TRP		38.752 -22.303 14.428 1.00 30.37	В
MOTA	1906	CA	TRP		37.790 -21.525 15.194 1.00 31.57 38.129 -20.024 15.140 1.00 32.14	B B
MOTA	1907	CB	TRP			В
MOTA	1908	CG	TRP		39.430 -19.666 15.824 1.00 33.73 40.359 -18.648 15.429 1.00 35.16	В
ATOM ATOM	1909 1910		2 TRP		41,418 -18.662 16.362 1.00 35.99	В
ATOM	1911		TRP			В
MOTA	1912		LTRP			В
MOTA	1913		1 TRP		41.142 -19.642 17.278 1.00 33.97	В
ATOM	1914		2 TRP		_	В
MOTA	1915		3 TRP			В
MOTA	1916		2 TRP			B
MOTA	1917		TRP			В
MOTA	1918		TRP ASN			В
MOTA	1919	N	MON	D 02	30,131 -21,333 13.444 1,00 31.03	~

ATOM	1920	CA	ASN :	В	62	34.781 -22.191 12.950 1.00 32.57	В
ATOM	1921	CB	ASN :		62	34.701 -22.021 11.434 1.00 30.37	В
ATOM	1922	CG	asn	В	62	34.575 -20.574 11.025 1.00 29.69	В
MOTA	1923		asn :		62	33.889 -19.794 11.680 1.00 29.42	В
MOTA	1924		ASN		62	35.222 -20.209 9.926 1.00 31.50	В
MOTA	1925	C	ASN		62	34.238 -23.561 13.339 1.00 32.87	В
MOTA MOTA	1926	0	asn ser		62 63	33.028 -23.789 13.292 1.00 34.70 35.128 -24.469 13.725 1.00 32.43	B
ATOM	1927 1928	N CA	SER		63	34.705 -25.797 14.140 1.00 32.38	В
ATOM	1929	CB	SER		63	35.818 -26.819 13.879 1.00 32.20	В
ATOM	1930	OG	SER		63	36.905 -26.626 14.760 1.00 33.33	В
MOTA	1931	C	SER		63	34.348 -25.768 15.630 1.00 32.14	В
MOTA	1932	0	SER	В	63	33.677 -26.667 16.138 1.00 32.86	В
MOTA	1933	N	GLN	В	64	34.794 -24.724 16.325 1.00 31.10	В
ATOM	1934	CA	GLN	В	64	34.513 -24.569 17.752 1.00 30.99	В
MOTA	1935	CB	GLN		64	35.661 -23.837 18.446 1.00 32.54	В
ATOM	1936	CG	GTM		64	36.988 -24.557 18.383 1.00 34.49	В
ATOM	1937	co	GLN		64	36.870 -25.998 18.810 1.00 38.20	B
ATOM ATOM	1938 1939		GLN		64 64	36.629 -26.884 17.984 1.00 40.82 37.022 -26.245 20.108 1.00 38.34	В
MOTA	1940	C	GLN		64	33.226 -23.775 17.944 1.00 29.88	В
MOTA	1941	ō	GLN		64	33.252 -22.549 18.064 1.00 29.28	В
ATOM	1942	N	LYS		65	32.101 -24.476 17.979 1.00 28.74	В
ATOM	1943	CA	LYS		65	30.815 -23.812 18.123 1.00 29.18	В
ATOM	1944	CB	LYS	В	65	29.688 -24.851 18.132 1.00 30.63	В
MOTA	1945	CG	LYS	В	65	29.575 -25.612 16.812 1.00 32.20	В
MOTA	1946	æ	LYS		65	29.371 -24.654 15.629 1.00 34.44	В
MOTA	1947	CE	LYS		65	29.688 -25.327 14.284 1.00 37.24	В
MOTA	1948	NZ	LYS		65	29.430 -24.427 13.109 1.00 37.89	В
MOTA	1949	C	LYS		65 65	30.745 -22.919 19.352 1.00 28.19 30.075 -21.891 19.333 1.00 28.16	B B
MOTA MOTA	1950 1951	N O	LYS ASP		65 66	31.440 -23.304 20.417 1.00 27.58	В
ATOM	1952	CA	ASP		66	31.460 -22.504 21.636 1.00 27.41	В
ATOM	1953	CB	ASP		66	32.283 -23.208 22.727 1.00 28.45	В
ATOM	1954	CG	ASP		66	33.559 -23.847 22.184 1.00 32.24	В
MOTA	1955		ASP		66	33.478 -24.591 21.183 1.00 33.17	В
ATOM	1956		ASP		66	34.642 -23.623 22.765 1.00 33.25	В
MOTA	1957	C	ASP	В	66	32.050 -21.131 21.316 1.00 26.63	В
MOTA	1958	0	ASP		66	31.468 -20.102 21.662 1.00 24.32	В
MOTA	1959	N	ILE		67	33.198 -21.116 20.640 1.00 26.12	В
ATOM	1960	CA	ILE		67	33.840 -19.855 20.273 1.00 26.42	B B
ATOM	1961	CB	ILE		67 67	35.206 -20.088 19.613 1.00 28.29 35.859 -18.753 19.290 1.00 28.54	В
ATOM ATOM	1962 1963		ILE		67	36.094 -20.925 20.535 1.00 28.25	В
ATOM	1964		ILB		67	36.319 -20.321 21.906 1.00 32.66	В
ATOM	1965	c	ILE		67	32.968 -19.061 19.300 1.00 26.36	В
ATOM	1966	0	ILE		67	32.747 -17.869 19.491 1.00 25.33	В
MOTA	1967	N	LEU	В	68	32.472 -19.730 18.261 1.00 26.11	В
MOTA	1968	CA	LEU		68	31.617 -19.086 17.267 1.00 26.66	В
MOTA	1969	CB	Pea		68	31.132 -20.102 16.235 1.00 27.61	В
MOTA	1970	CG	LEU		68	31.807 -20.171 14.872 1.00 30.12	В
MOTA	1971		LEU		68	31.081 -21.216 14.031 1.00 33.09	В
MOTA	1972		PEA		68 68	31.766 -18.812 14.190 1.00 30.01 30.394 -18.415 17.878 1.00 26.81	B
MOTA MOTA	1973 1974	С 0	PEA PEA		68	30.067 -17.280 17.541 1.00 26.19	В
ATOM	1975	И	GLU		69	29.706 -19.135 18.756 1.00 28.87	В
ATOM	1976	CA	GLU		69	28.509 -18.614 19.404 1.00 31.55	В
ATOM	1977	СВ	GLU		69	27.945 -19.654 20.382 1.00 35.75	В
MOTA	1978	CG	GLU	В	69	27.304 -20.862 19.695 1.00 43.71	В
MOTA	1979	æ	GLU		69	26.883 -21.954 20.673 1.00 47.92	В
MOTA	1980		. GLU		69	27.756 -22.454 21.418 1.00 49.27	В
MOTA	1981		GLU		69	25.683 -22.316 20.694 1.00 50.44	В
MOTA	1982	C	GLU		69	28.773 -17.295 20.130 1.00 29.82	В
MOTA	1983	0	GLU		69 70	27.986 -16.356 20.027 1.00 27.91 29.886 -17.226 20.855 1.00 29.32	B B
MOTA	1984	N	ARG ARG		70	30.239 -16.016 21.597 1.00 28.97	В
MOTA MOTA	1985 1986	CA CB	ARG		70	31.347 -16.315 22.606 1.00 28.94	В
ATOM	1986	CG	ARG		70	30.982 -17.344 23.673 1.00 30.55	В
ATOM	1988	CD	ARG		70	32.251 -17.810 24.371 1.00 32.35	В
ATOM	1989	NE	ARG		70	32.040 -19.037 25.117 1.00 34.83	В
ATOM	1990	CZ	ARG	В	70	32.946 -19.997 25.232 1.00 34.98	В
MOTA	1991		L ARG		70	34.131 -19.875 24.647 1.00 35.03	В
MOTA	1992		ARG		70	32.662 -21.083 25.930 1.00 39.48	В
MOTA	1993	C	ARG	В	70	30.691 -14.888 20.682 1.00 26.77	В

ATOM	1994	0	ARG	В	70	30.412	-13.725	20.951	1.00 26.95	В
ATOM	1995	N	LYS	В	71	31.395	-15.235	19.608	1.00 25.97	В
MOTA	1996	CA	LYS		71	31.885		18.670	1.00 25.98	В
ATOM	1997	CB	LYS		71	32.830		17.652	1.00 27.62	В
ATOM	1998	CG	LYS		71	33.728		16.924	1.00 29.24 1.00 32.14	В
ATOM	1999	CD CD	LYS		71	34.628		17.909 17.236	1.00 32.14	B B
MOTA MOTA	2000 2001	CE NZ	LYS		71 71	35.430	-12.035	18.245	1.00 34.18	В
ATOM	2002	C	LYS		71		-13.591	17.952	1.00 25.22	В
ATOM	2003	ō	LYS		71		-12.395	17.671	1.00 24.39	В
ATOM	2004	N	ARG		72	29.701	-14.399	17.657	1.00 25.08	В
MOTA	2005	CA	ARG	В	72	28.500	-13.922	16.989	1.00 26.32	В
MOTA	2006	CB	ARG	В	72	27.628	-15.101	16.561	1.00 28.02	В
ATOM	2007	CG	ARG		72		-15.830	15.340	1.00 28.10	В
MOTA	2008	CD	ARG		72		-17.013	15.083	1.00 32.02	В
MOTA	2009	NE	ARG		72		-17.583	13.766	1.00 36.46 1.00 38.62	B B
MOTA	2010	CZ	ARG ARG		72 72		-18.779 -19.538	13.389 14.238	1.00 37.88	В
MOTA MOTA	2011 2012		ARG		72		-19.338	12.163	1.00 37.00	В
ATOM	2013	C	ARG		72		-13.017	17.898	1.00 24.31	В
MOTA	2014	ō	ARG		72		-12.326	17.439	1.00 24.84	В
ATOM	2015	N	ALA		73	27.990	-13.028	19.189	1.00 26.18	В
MOTA	2016	CA	ALA	В	73	27.267	-12.185	20.140	1.00 28.18	В
MOTA	2017	CB	ALA		73		-12.974	21.418	1.00 28.97	В
MOTA	2018	С	ALA		73		-10.916	20.472	1.00 28.97	В
MOTA	2019	0	ALA			27.528	-9.977	21.066	1.00 30.50	B B
ATOM	2020	N	ALA	_	74		-10.882 -9.732	20.070 20.347	1.00 29.65 1.00 30.77	В
ATOM ATOM	2021 2022	CA CB	ALA ALA		74 74	30.170 31.558	-9.752	19.764	1.00 30.77	В
MOTA	2022	C	ALA		74	29.594	-8.414	19.827	1.00 31.78	В
ATOM	2024	ō	ALA		74	29.789	-7.359	20.438	1.00 32.74	В
ATOM	2025	N	VAL		75	28.886	-8.465	18.704	1.00 31.60	В
ATOM	2026	CA	VAL	В	75	28.308	-7.248	18.145	1.00 32.38	В
MOTA	2027	CB	VAL	В	75	27.397	-7.539	16.929	1.00 30.51	В
MOTA	2028		VAL		75	27.291	-6.295	16.062	1.00 31.44	В
MOTA	2029		VAL		75	27.931	-8.696	16.137	1.00 33.08	В
MOTA	2030	C	VAL		75 75	27.465	-6.529	19.201	1.00 33.07 1.00 33.54	B B
ATOM	2031	o N	VAL ASP		75 76	27.402 26.811	-5.302 -7.302	19.218 20.065	1.00 34.70	В
MOTA MOTA	2032 2033	CA.	ASP		76 76	25.971	-6.748	21.130	1.00 36.27	В
ATOM	2033	CB	ASP		76	24.780	-7.670	21.420	1.00 38.57	В
MOTA	2035	CG	ASP		76	23.889	-7.881	20.215	1.00 41.48	В
ATOM	2036	OD1	ASP	В	76	23.335	-6.887	19.694	1.00 43.46	В
MOTA	2037	OD2	ASP	В	76	23.739	-9.048	19.792	1.00 43.76	В
MOTA	2038	C	ASP		76	26.780	-6.600	22.411	1.00 35.56	В
MOTA	2039	0	ASP		76	26.731	-5.569	23.081	1.00 34.13	В
MOTA	2040	N	ARG		77	27.508	-7.661	22.744	1.00 35.22 1.00 34.49	B B
MOTA	2041	CA	ARG		77 77	28.343	-7.708 -9.052	23.937 23.991	1.00 34.49	В
MOTA	2042 2043	CB CG	ARG		77 77	29.071 29.841	-9.328	25.271	1.00 40.90	В
ATOM ATOM	2043	CD	ARG		77		-10.553	25.102	1.00 43.79	В
ATOM	2045	NE	ARG		77		-11.743	24.665	1.00 48.65	В
ATOM	2046	CZ	ARG		77		-12.385	25.406	1.00 51.36	В
ATOM	2047	NH1	. ARG	В	77	28.816	-11.949	26.626	1.00 52.34	В
MOTA	2048	NH2	ARG		77		-13.470	24.935	1.00 50.76	В
MOTA	2049	C	ARG		77	29.362		23.927	1.00 32.18	В
MOTA	2050	0	ARG		77	29.499		24.896	1.00 32.49	В
MOTA	2051	N	VAL		78	30.073 31.086		22.818	1.00 30.66 .1.00 29.00	B B
MOTA MOTA	2052 2053	CA CB	VAI VAI		78 78	32.276		21.867	1.00 27.82	В
MOTA	2054		VAI		78	33.327		21.740	1.00 25.08	В
ATOM	2055		VAL		78	32.870			1.00 23.27	В
ATOM	2056	С	VAI		78	30.594		22,113	1.00 29.33	В
ATOM	2057	0	VAI		78	30.435		22.831	1.00 29.83	В
MOTA	2058	N	CYS		79	30.354		20.804	1.00 28.42	В
ATOM	2059	CA	CYS		79	29.927		20.083	1.00 29.14	В
ATOM	2060	C	CYS		79	28.724		20.629	1.00 28.59	В
MOTA	2061	O	CYS		79 70	28.883		21.062 18.604	1.00 26.06 1.00 29.19	B B
MOTA	2062 2063	CB SG	CYS		79 79	29.675 31.052		17.680	1.00 23.13	В
ATOM ATOM	2064	Ŋ	ARC		80	27.527		20.586	1.00 28.34	В
ATOM	2065	CA	ARC		80	26.347		21.071	1.00 30.77	В
ATOM	2066	CB	ARC		80	25.079		20.915	1.00 32.82	В
ATOM	2067	CG		3 B	80	24.612		19.474	1.00 35.65	В

ATOM	2068	CD	ARG	В	80	23.120	-3.273	19.387	1.00 36.01	В
MOTA	2069	NE	ARG	В	80	22.649	-3.243	18.005	1.00 35.49	В
ATOM	2070	CZ	ARG	В	80	22.913	-4.188	17.108	1.00 37.80	В
ATOM	2071	NH1	ARG	В	80	23.640	-5.242	17.449	1.00 40.57	В
ATOM	2072	NH2	ARG	В	80	22.467	-4.075	15.864	1.00 38.86	В
ATOM	2073	C	ARG		80	26.507	-1.552	22.524	1.00 31.24	В
ATOM	2074	ō	ARG		80	25.975	-0.525	22.944	1.00 32.07	В
ATOM	2075	N	HIS		81	27.257	-2.337	23.283	1.00 31.40	В
ATOM	2076	CA	HIS		81	27.492	-2.028	24.683	1.00 32.20	В
ATOM	2077	CB	HIS		81	28.220	-3.185	25.366	1.00 33.00	В
ATOM	2078	CG	HIS		81	28.595	-2.899	26.787	1.00 37.24	B
					81	29.764	-2.490	27.335	1.00 37.24	В
ATOM	2079		HIS				-2.981		1.00 39.11	В
ATOM	2080		HIS		81	27.692		27.826		
ATOM	2081		HIS		81	28.290	-2.635	28.952	1.00 40.49	В
ATOM	2082		HIS	_	81	29.548	-2.332	28.682	1.00 39.16	В
ATOM	2083	C	HIS		81	28.326	-0.762	24.831	1.00 30.87	В
ATOM	2084	0	HIS		81	27.906	0.206	25.470	1.00 31.38	В
ATOM	2085	N	asn		82	29.511	-0.770	24.233	1.00 29.77	В
MOTA	2086	CA	asn	В	82	30.403	0.375	24.332	1.00 28.02	В
MOTA	2087	CB	asn	В	82	31.755	0.056	23.683	1.00 26.64	В
ATOM	2088	CG	ASN	В	82	32.470	-1.092	24.373	1.00 25.02	В
ATOM	2089	OD1	ASN	В	82	32.305	-1.305	25.572	1.00 24.06	В
MOTA	2090	ND2	ASN	В	82	33.278	-1.829	23.619	1.00 26.38	В
ATOM	2091	C	ASN	В	82	29.819	1.648	23.741	1.00 26.04	В
ATOM	2092	Ō	ASN		82	30.163	2.747	24.174	1.00 25.71	В
ATOM	2093	N	TYR		83	28.930	1.512	22.765	1.00 25.90	В
ATOM	2094	CA	TYR		83	28.324	2.693	22.156	1.00 25.91	В
ATOM	2095	CB	TYR		83	27.462	2.297	20.946	1.00 25.69	В
ATOM	2096	CG	TYR		83	27.102	3.462	20.056	1.00 25.95	В
			TYR		83	26.022	4.294	20.353	1.00 27.11	В
ATOM	2097		TYR		83	25.712	5.403	19.545	1.00 25.98	В
MOTA	2098		TYR		83	27.865	3.759	18.933	1.00 27.72	В
ATOM	2099							18.121	1.00 28.05	В
ATOM	2100		TYR		83	27.567	4.862			В
MOTA	2101	CZ	TYR		83	26.493	5.680	18.434	1.00 27.73	
MOTA	2102	OH	TYR		83	26.225	6.781	17.645	1.00 27.55	В
ATOM	2103	С	TYR		83	27.485	3.458	23.181	1.00 25.87	В
MOTA	2104	0	TYR		83	27.315	4.673	23.070	1.00 26.05	В
MOTA	2105	N	GLN	В	84	26.975	2.750	24.186	1.00 28.25	В
MOTA	2106	CA	GLN	В	84	26.159	3.375	25.229	1.00 30.44	B
ATOM	2107	CB	GLN	В	84	25.467	2.310	26.093	1.00 34.30	В
MOTA	2108	CG	GLN	В	84	24.595	1.343	25.301	1.00 40.52	В
ATOM	2109	CD	GLN	В	84	23.515	2.047	24.496	1.00 43.21	В
MOTA	2110	OE1	GLN	В	84	23.023	1.516	23.499	1.00 46.12	В
ATOM	2111	NE2	GLN	В	84	23.133	3.244	24.932	1.00 45.41	В
MOTA	2112	C	GLN	В	84	27.030	4.254	26.111	1.00 29.01	В
ATOM	2113	0	GLN	В	84	26.633	5.353	26.494	1.00 27.82	В
ATOM	2114	N	LEU		85	28.219	3.757	26.436	1.00 28.32	В
ATOM	2115	CA	LEU		85	29.150	4.505	27.263	1.00 28.76	В
ATOM	2116	СВ	LEU		85	30.355	3.631	27.631	1.00 28.92	В
ATOM	2117	CG	LEU		85	30.065	2,226	28.184	1.00 30.98	В
ATOM	2118		. LEU		85	31.343	1.631	28.758	1.00 30.59	В
	2119		LEU		85	29.006	2.291	29.265	1.00 31.87	В
MOTA MOTA	2120	C	LEU		85	29.609	5.719	26.461	1.00 29.95	В
	2121		LEU		85	29.836	6.798	27.010	1.00 30.93	В
ATOM		0					5.529	25.150	1.00 30.31	В
MOTA	2122	N	GLU		86	29.724		24.245	1.00 31.41	В
ATOM	2123	CA	GLU		86	30.160	6.577		1.00 32.60	В
MOTA	2124	CB	· GLU		86	30.426	5.981	22.861		
MOTA	2125	CG	GLU		86	31.741	6.420	22.236	1.00 39.25	В
MOTA	2126	CD	GLU		86	32.962	5.854	22.953	1.00 41.02	В
MOTA	2127		L GLU		86	33.379	4.714	22.636	1.00 40.75	В
MOTA	2128	OE	GLU	В	86	33.497	6.553	23.843	1.00 41.96	В
MOTA	2129	C	GLU	В	86	29.113	7.684	24.146	1.00 32.44	В
MOTA	2130	0	GLU	В	86	29.454	8.865	24.109	1.00 30.73	В
ATOM	2131	N	TEC	В	87	27.838	7.303	24.103	1.00 33.77	В
ATOM	2132	CA	LEU	В	87	26.755	8,282	24.015	1.00 34.65	В
MOTA	2133	CB	TR(87	25.398	7.583	23.899	1.00 34.69	В
ATOM	2134	CG	LEC		87	24.916	7.169	22.508	1.00 36.86	В
ATOM	2135		L LEC		87	23.655	6.326	22.642	1.00 35.43	В
ATOM	2136		2 LET		87	24.645	8.411	21.660	1.00 35.76	В
ATOM	2137	c c	LEU		87	26.740	9.199	25.231	1.00 35.16	В
ATOM	2138	ō	LEC			26.250	10.326	25.164	1.00 34.29	В
ATOM	2139	N	ARC			27.280	8.711	26.343	1.00 36.69	В
ATOM	2140					27.200	9.493	27.573	1.00 37.64	В
	2140			3 B		27.173	8.575	28.791	1.00 39.79	В
ATOM	マイダエ	هب	ALC:		30	61,113	0.575	~~.,,_		_

ATOM	2142	CG	ARG	В	88	25.827	7.878	28.908	1.00 45.19	В
ATOM	2143	CD	ARG		88	25.704	7.173	30.253	1.00 49.04	В
ATOM	2144	NE	ARG		88	26.657	6.074	30.388	1.00 54.57	В
MOTA	2145	CZ	ARG		88	27.101	5.603	31.552	1.00 55.76	В
MOTA	2146	NH1	arg	В	88	26.683	6.137	32.694	1.00 55.56	В
ATOM	2147	NH2	ARG	В	88	27.963	4.595	31.574	1.00 56.11	В
ATOM	2148	C	ARG		88	28.601	10.299	27.714	1.00 36.93	В
	2149					28.702				
ATOM		0	ARG		88		11.160	28.589	1.00 37.24	В
ATOM	2150	N	THR		89	29.571	10.035	26.842	1.00 35.19	В
MOTA	2151	CA	THR	В	89	30.860	10.712	26.914	1.00 31.71	В
ATOM	2152	CB	THR	В	89	31.916	9.767	27.529	1.00 31.61	В
MOTA	2153	OG1	THR	В	89	31.980	8.554	26.762	1.00 29.72	В
ATOM	2154	CG2	THR		89	31.557	9.436	28.963	1.00 25.87	В
ATOM	2155	C	THR		89	31.420	11.254	25.600	1.00 31.31	В
MOTA	2156	0	THR		89	31.214	12.415	25.249	1.00 32.41	В
MOTA	2157	N	THR	В	90	32.139	10.403	24.880	1.00 30.72	В
ATOM	2158	CA	THR	В	90	32.766	10.786	23.623	1.00 30.43	В
ATOM	2159	СВ	THR	В	90	33.368	9.558	22.925	1.00 30.54	В
ATOM	2160		THR		90	34.297	8.919	23.808	1.00 33.70	В
										В
ATOM	2161	CG2	THR		90	34.099	9.970	21.666	1.00 31.65	
ATOM	2162	С	THR	В	90	31.874	11.512	22.625	1.00 30.61	, B
ATOM	2163	0	THR	В	90	32.267	12.543	22.070	1.00 30.24	В
ATOM	2164	N	LEU	В	91	30.683	10.977	22.385	1.00 30.30	В
ATOM	2165	CA	LEU	В	91	29.767	11.581	21.425	1.00 31.93	В
ATOM	2166	СВ	LEU		91	28.709	10.554	21.007	1.00 32.55	В
										В
ATOM	2167	CG	PEA		91	29.268	9.315	20.292	1.00 33.01	
MOTA	2168		LEU		91	28.201	8.233	20.205	1.00 33.73	В
MOTA	2169	CD2	LEU	В	91	29.761	9.700	18.902	1.00 31.26	В
ATOM	2170	С	LEU	В	91	29.096	12.872	21.907	1.00 32.38	В
ATOM	2171	0	LEU	В	91	28.402	13.534	21.139	1.00 32.08	В
ATOM	2172	Ŋ	GLN		92	29.303	13.229	23.173	1.00 32.44	В
									1.00 34.54	
MOTA	2173	CA	GLN		92	28.725	14.454	23.713		В
MOTA	2174	CB	GLN		92	28.138	14.217	25.110	1.00 38.48	В
MOTA	2175	CG	GTM	В	92	26.836	13.419	25.121	1.00 44.66	В
MOTA	2176	CD	GLN	В	92	26.233	13.291	26.516	1.00 49.27	В
ATOM	2177	OB1	GLN	В	92	25.239	12.588	26.712	1.00 51.65	В
ATOM	2178	NE2	GLN		92	26.832	13.975	27.491	1.00 49.93	В
										• в
MOTA	2179	C	GLN		92	29.779	15.557	23.777	1.00 32.86	
MOTA	2180	0	GLN		92	29.457	16.721	24.019	1.00 32.19	В
ATOM	2181	N	ARG	В	93	31.038	15.187	23.555	1.00 31.53	В
MOTA	2182	CA	ARG	В	93	32.132	16.157	23.576	1.00 29.87	В
ATOM	2183	СВ	ARG		93	33.477	15.472	23.302	1.00 28.14	В
ATOM	2184	CG	ARG		93	34.681	16.433	23.217	1.00 23.56	В
							15.656	22.925	1.00 22.53	В
ATOM	2185	CD	ARG		93	35.953				
MOTA	2186	NE	ARG		93	37.128	16.486	22.662	1.00 19.19	В
ATOM	2187	CZ	ARG	В	93	37.769	17.205	23.581	1.00 18.66	В
ATOM	2188	NH1	ARG	В	93	37.352	17.214	24.843	1.00 17.45	В
ATOM	2189	NH2	ARG	В	93	38.847	17.898	.23.242	1.00 16.56	В
MOTA	2190	C	ARG	В	93	31.921	17.245	22.535	1.00 29.02	В
ATOM	2191	ō	ARG		93	31.755	16.965	21.349	1.00 29.55	В
ATOM			ARG			31.933	18.490	22.987	1.00 28.71	В
	2192	N			94					
ATOM	2193	CA	ARG		94	31.767	19.613	22.087	1.00 29.63	В
MOTA	2194	CB	ARG	В	94	30.299	20.046	22.041	1.00 32.44	В
MOTA	2195	CG	ARG	В	94	29.506	19.196	21.060	1.00 37.10	В
ATOM	2196	CD	ARG	В	94	28.016	19.414	21.124	1.00 39.80	В
MOTA	2197	NE	ARG		94	27,350	18.742	20.008	1.00 44.04	В
ATOM	2198	cz	ARG		94	27.372	17.428	19.791	1.00 44.11	В
ATOM	2199		ARG		94	28.026	16.625	20.617	1.00 45.60	В
ATOM	2200		ARG		94	26.747	16.916	18.739	1.00 44.45	В
ATOM	2201	С	ARG	В	94	32.656	20.760	22.498	1.00 28.84	В
MOTA	2202	0	ARG	В	94	32.464	21.363	23.550	1.00 29.13	В
MOTA	2203	N	VAL	В	95	33.650	21.038	21.663	1.00 27.49	В
ATOM	2204	CA	VAL		95	34.592	22.117	21.916	1.00 26.47	В
ATOM	2205	CB	VAL		95	36.047	21.605	21.890	1.00 25.65	В
MOTA	2206		VAL		95	37.004	22.734	22.260	1.00 22.82	В
ATOM	2207		VAL		95	36.202	20.423	22.849	1.00 26.01	В
MOTA	2208	C	VAL	В	95	34.415	23.180	20.840	1.00 27.00	В
MOTA	2209	0	VAL	В	95	34.721	22.945	19.665	1.00 27.00	В
MOTA	2210	N	GLU		96	33.912	24.340	21.253	1.00 26.94	В
ATOM	2211	CA	GLU		96	33.673	25.462	20.348	1.00 26.50	В
		CB						21.107	1.00 29.19	В
ATOM	2212		GLU		96	33.072	26.649			
MOTA	2213	CG	GLU		96	31.736	26.372	21.775	1.00 36.47	В
MOTA	2214	Э	GLU		96	31.211	27.582	22.537	1.00 40.45	В
MOTA	2215	OE1	. GLU	В	96	30.121	27.477	23.144	1.00 42.85	В

MOTA 2216 OE2 GLU B 96 31.891 28.634 22.526 1.00 40.11 В GLU B 96 34.960 25.916 19.689 1.00 25.02 MOTA 2217 C 26.022 ATOM 2218 0 GLU B 96 35,999 20.338 1.00 24.73 MOTA 2219 N PRO B 97 34.900 26.204 18.383 1.00 24.54 MOTA 2220 CD PRO B 97 33.744 26.011 17.493 1.00 22.89 36.069 26.655 17.626 1.00 23.87 PRO B 97 MOTA 2221 CA 35.580 26.633 16.175 1.00 22.81 MOTA 2222 CB PRO B 97 В PRO B 97 34.411 25.663 16.202 1.00 25.55 ATOM 2223 CG 1.00 23.80 ATOM PRO B 97 36.498 28.061 18.021 2224 С 35.665 28.905 1.00 24.40 PRO B 97 18.353 ATOM 2225 0 1.00 22.02 ATOM 2226 N THR B 98 37.799 28.307 17.990 В ATOM 2227 CA THR B 98 38.306 29.634 18.266 1.00 24.00 В THR B 98 39.569 29.592 19.150 1.00 27.31 CB ATOM 2228 OG1 THR B 98 40.626 28.929 18.449 1.00 35.69 В ATOM 2229 1.00 26.76 CG2 THR B 98 39.282 28.839 20.439 В ATOM 2230 38.631 30.143 16.860 1.00 22.38 MOTA 2231 С THR B 98 В THR B 98 39.376 29.504 16.116 1.00 19.48 ATOM 2232 0 1.00 21.55 VAL B 99 38.041 31,274 16.487 MOTA 2233 N 15.152 1.00 21.20 VAL B 99 38.242 31.824 В MOTA 2234 CA 36.871 32.153 14.509 1.00 21.09 R MOTA 2235 CB VAL B 99 CG1 VAL B 99 37.043 32.541 13.050 1.00 19.62 MOTA 2236 35.950 30.944 14.625 1.00 18.29 CG2 VAL B 99 ATOM 2237 15.167 1.00 21.59 VAL B 99 39.140 33.059 В MOTA 2238 C VAL B 99 38.970 33.962 15.982 1.00 21.57 В ATOM 2239 0 1.00 22.65 ATOM THR B 100 40.099 33.084 14.252 2240 N 14.168 1.00 24.95 ATOM 2241 CA THR B 100 41.056 34.179 14.820 1.00 26.31 THR B 100 42.399 33.770 В ATOM 2242 CB 42.162 MOTA 2243 OG1 THR B 100 33.321 16.160 1.00 30.10 В 43.359 34.942 14.854 1.00 29.07 CG2 THR B 100 MOTA 2244 41.329 34.556 12.717 1.00 24.61 R MOTA 2245 THR B 100 C MOTA 2246 THR B 100 41.514 33.689 11.869 1.00 23.89 ILE B 101 41.363 35.852 12.435 1.00 26.18 2247 MOTA N 36.315 11.080 1.00 29.32 41.638 MOTA 2248 CA ILE B 101 1.00 29.37 10.582 40.572 MOTA 2249 CB ILE B 101 37.327 9.231 1.00 29.49 ATOM 2250 CG2 ILE B 101 40.986 37.885 В 36.664 10.492 1.00 30.11 В CG1 ILE B 101 39.198 MOTA 2251 38.110 37.605 10.002 1.00 29.81 CD1 ILE B 101 MOTA 2252 42.988 37.015 11.040 1.00 31.04 2253 ILE B 101 MOTA С ILE B 101 43.270 37.868 11.877 1.00 31.24 В MOTA 2254 0 43.820 36.664 10.066 1.00 34.47 SER B 102 ATOM 2255 N 45,124 37.303 9.940 1.00 39.17 MOTA 2256 CA **SER B 102** 2257 **SER B 102** 46.143 36.617 10.844 1.00 37.33 В ATOM CB 46.326 35.265 10.462 1.00 41.93 B MOTA 2258 OG **SER B 102** SER B 102 45.632 37.289 8.501 1.00 42.45 В ATOM 2259 C 7.845 1.00 42.45 45.641 36.248 ATOM 2260 0 **SER B 102** 46.052 38.455 7.988 1.00 45.38 В PRO B 103 ATOM 2261 45.938 39.793 8.596 1.00 45.47 В MOTA 2262 CD PRO B 103 1.00 48.91 B PRO B 103 46.564 38.545 6.617 2263 ATOM CA 46.446 ATOM 40.032 6.312 1.00 47.74 В 2264 CB PRO B 103 7.642 1.00 47.08 46.739 40.652 2265 PRO B 103 ATOM CG 1.00 51.96 В MOTA 2266 C PRO B 103 48.010 38.042 6.545 48.688 37.957 7.568 1.00 52.51 В ATOM 2267 0 PRO B 103 48.475 37.699 5.346 1.00 55.84 SER B 104 MOTA 2268 N 1.00 60.00 49.843 37.209 5.177 MOTA 2269 CA **SER B 104** 1.00 59.60 SER B 104 50.018 36.578 3.791 ATOM 2270 CB OG **SER B 104** 49.778 37.520 2.759 1.00 59.05 ATOM 2271 50.842 38.353 5.368 1.00 63.75 В SER B 104 ATOM C 2272 1.00 64.64 50.853 39.325 4.605 ATOM 2273 ٥ SER B 104 В 1.00 66.99 ATOM 2274 N ARG B 105 51.677 38.228 6.398 52.674 39.242 6.736 1.00 69.17 В MOTA 2275 CA ARG B 105 1.00 70.33 53.631 38.700 7.808 ARG B 105 ATOM 2276 CB 1.00 72.24 54.672 37.690 7.318 MOTA 2277 CG ARG B 105 1.00 73.51 54.073 36.586 6.449 MOTA 2278 œ ARG B 105 52.981 35.859 7.095 1.00 75.02 В ARG B 105 NE MOTA 2279 В 53.120 35.051 8.142 1.00 76.07 ATOM 2280 CZ ARG B 105 1.00 77.38 ATOM NH1 ARG B 105 54.314 34.852 8.684 2281 1.00 76.05 ATOM 2282 NH2 ARG B 105 52.059 34.431 8.644 39.720 5.523 1.00 70.38 В ARG B 105 53.464 ATOM 2283 C В 53.134 40.746 4.923 1.00 71.56 MOTA 2284 O ARG B 105 46.629 1.00 49.25 В 40.478 -1.867 MOTA 2285 **ASN B 113** N 1.00 48.42 46.963 40.039 -0.515 ATOM 2286 CA **ASN B 113** В 46.726 41.181 0.477 1.00 51.23 ATOM 2287 CB **ASN B 113** В 47.268 40.875 1.863 1.00 53.89 ATOM CG **ASN B 113** 2288 48.429 40.498 2.019 1.00 55.14 MOTA 2289 OD1 ASN B 113

ATOM	2290	ND2	ASN E	3 113	46.428	41.048	2.880	1.00 55.30	В
MOTA	2291	C	ASN E	3 213	46.143	38.808	-0.118	1.00 45.78	В
ATOM	2292	ō	ASN I		45.155	38.471	-0.774	1.00 44.99	В
MOTA	2293	N	LEU I		46.550	38.146	0.961	1.00 42.27	В
MOTA	2294	CA	PRO E		45.862	36.944	1.415	1.00 38.77	В
ATOM	2295	CB	TEO E	3 114	46.770	35.739	1.182	1.00 39.10	В
ATOM	2296	CG	TEA B	3 114	46.238	34.330	1.421	1.00 40.81	В
ATOM	2297	CD1	LEU E	3 114	45.097	34.023	0.459	1.00 41.59	В
ATOM	2298	CD2	LEU I	3 114	47.379	33.341	1.222	1.00 41.03	В
ATOM	2299	C	LEU I		45.424	36.986	2.883	1.00 36.39	В
MOTA		ŏ					3.783	1.00 35.98	В
	2300		LEU I		46.237	37.204			
ATOM	2301	N	LEU I		44.130	36.777	3.112	1.00 31.79	В
MOTA	2302	CA	TEO I	B 115	43.576	36.766	4.460	1.00 28.77	В
MOTA	2303	CB	TEO 1	B 115	42.231	37.496	4.493	1.00 29.52	В
ATOM	2304	CG	LEU I	B 115	42.156	38.843	5.218	1.00 30.12	В
ATOM	2305	CD1	TEG 1	B 115	43.281	39.751	4.764	1.00 30.28	В
ATOM	2306	CD2	PEO 1		40.799	39.479	4.951	1.00 28.39	В
	2307	C	TEO I		43.374	35.323	4.896	1.00 27.23	В
ATOM									
ATOM	2308	0	TEO 1		42.815	34.513	4.154	1.00 25.72	В
MOTA	2309	N	VAL I		43.825	35.002	6.103	1.00 24.13	В
ATOM	2310	CA	VAL 1	B 116	43.695	33.651	6.618	1.00 20.76	В
MOTA	2311	CB	VAL 1	B 116	45.078	33.098	7.078	1.00 20.02	В
ATOM	2312	CG1	VAL 1	B 116	44.915	31.757	7.777	1.00 17.46	В
ATOM	2313	CG2	VAL 1	B 116	45.996	32.944	5.880	1.00 19.44	В
ATOM	2314	c	VAL 1		42.723	33.568	7.784	1.00 20.38	В
				B 116			8.766	1.00 19.54	В
ATOM	2315	0			42.860	34.293			
ATOM	2316	N		B 117	41.724	32.701	7.669	1.00 20.87	В
MOTA	2317	CA	CYS	B 117	40.793	32.523	8.774	1.00 22.57	В
MOTA	2318	C	CYS 1	B 117	41.132	31.196	9.444	1.00 21.84	В
ATOM	2319	0	CYS I	B 117	40.867	30.123	8.892	1.00 22.98	В
MOTA	2320	CB	CYS I	B 117	39.332	32.486	8.315	1.00 23.53	В
ATOM	2321	SG		B 117	38.217	32.222	9.734	1.00 29.76	В
ATOM				B 118	41.728	31.277	10.627	1.00 19.87	В
	2322	N							
MOTA	2323	CA		B 118	42.094	30.092	11.381	1.00 18.65	В
MOTA	2324	CB		B 118	43.345	30.356	12.226	1.00 19.67	В
MOTA	2325	OG	SER	B 118	44.463	30.672	11.421	1.00 22.97	В
ATOM	2326	С	SER	B 118	40.962	29.656	12.300	1.00 18.03	В
ATOM	2327	0	SER I	B 118	40.579	30.389	13.209	1.00 19.82	В
MOTA	2328	N		B 119	40.426	28.463	12.050	1.00 17.57	В
ATOM	2329	CA		B 119	39.365	27.889	12.874	1.00 15.30	В
		CB		B 119	38.202	27.364	12.006	1.00 15.69	В
ATOM	2330								В
ATOM	2331		VAL		37.091	26.852	12.892	1.00 11.64	
ATOM	2332		VAL :		37.695	28.484	11.076	1.00 13.82	В
MOTA	2333	С	VAL :	B 119	40.073	26.739	13.579	1.00 15.38	В
ATOM	2334	0	VAL :	B 119	40.318	25.680	12.992	1.00 16.76	В
MOTA	2335	N	THR	B 120	40.404	26.958	14.844	1.00 16.03	В
ATOM	2336	CA	THR	B 120	41.165	25.988	15.615	1.00 15.04	В
ATOM	2337	CB		B 120	42.487	26.613	16.031	1.00 13.75	В
ATOM	2338		THR		42.221	27.713	16.915	1.00 17.84	В
								1.00 12.18	В
ATOM	2339	CG2		B 120	43.230	27.144	14.815		
MOTA	2340	C		B 120	40.533	25.405	16.872	1.00 17.87	В
MOTA	2341	0		B 120	39.571	25.944			В
MOTA	2342	N	asp	B 121	41.132	24.303	17.317	1.00 19.07	В
ATOM	2343	CA	ASP	B 121	40.738	23.576	18.511	1.00 20.97	В
MOTA	2344	CB	ASP	B 121	41.268	24.291	19.766	1.00 24.82	В
ATOM	2345	CG		B 121	42.797	24.330	19.831	1.00 31.04	В
ATOM	2346		ASP		43.460	23.360	19,397	1.00 30.81	В
	2347			B 121	43.339	25.333	20.346	1.00 34.38	В
MOTA					39.238				В
MOTA	2348	C		B 121		23.293	18.679	1.00 21.27	
MOTA	2349	0		B 121	38.629	23.671	19.683	1.00 23.00	В
MOTA	2350	N	PHE	B 122	38.641	22.613	17.710	1.00 20.38	В
ATOM	2351	CA	PHE	B 122	37.233	22.280	17.818	1.00 18.51	В
MOTA	2352	CB	PHE	B 122	36.414	22.988	16.732	1.00 16.18	В
MOTA	2353	CG		B 122	36.817	22.644	15.319	1.00 13.31	В
ATOM	2354			B 122	37.695	23.463	14.615	1.00 11.43	В
ATOM	2355			B 122	36.247	21.547	14.664	1.00 10.93	В
									В
ATOM	2356			B 122	37.998	23.210	13.272	1.00 10.91	
MOTA	2357			B 122	36.541	21.280	13.317	1.00 12.31	В
ATOM	2358	CZ		B 122	37.419	22.118	12.618	1.00 8.92	В
MOTA	2359	C	PHE	B 122	37.011	20.778	17.739	1.00 19.55	В
MOTA	2360	0	PHB	B 122	37.889	20.029	17.301	1.00 18.45	В
ATOM	2361	N		B 123	35.829	20.357	18.182	1.00 20.50	В
ATOM	2362	CA		B 123	35.412	18.959	18.180	1.00 21.08	В
ATOM	2363	CB		B 123	36.067	18.201	19.340	1.00 19.11	В
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ATOM	2364	CG	TYR B :	123	35.919	16.702	19.228	1.00 18.56	В
ATOM	2365		TYR B		34.746	16.062	19.629	1.00 19.13	В
ATOM	2366	CB1	TYR B	123	34.572	14.695	19.446	1.00 17.75	В
MOTA	2367	CD2	TYR B	123	36.920	15.932	18.647	1.00 17.20	В
MOTA	2368	CE2	TYR B	123	36.762	14.566	18.455	1.00 17.38	В
ATOM	2369	CZ	TYR B	123	35.584	13.953	18.853	1.00 19.59	В
MOTA	2370	OH	TYR B		35.412	12.608	18.631	1.00 22.32	В
MOTA	2371	C	TYR B		33.896	18.957	18.351	1.00 21.83	В
MOTA	2372	0	TYR B		33.365	19.708	19.165	1.00 23.26	В
ATOM	2373	N	PRO B		33.175	18.126	17.584	1.00 21.65	В
MOTA	2374	CD	PRO B		31.725	17.996	17.808	1.00 23.81	В
ATOM	2375	CA	PRO B		33.627	17.177	16.562	1.00 22.30	В
ATOM	2376	СВ	PRO B		32.398	16.290	16.353	1.00 21.95 1.00 23.07	B B
ATOM	2377	CG	PRO B		31.270	17.237	16.586	1.00 23.07	В
ATOM	2378	C 0	PRO B		34.128 34.204	17.813 19.035	15.266 15.149	1.00 22.20	В
MOTA MOTA	2379 2380	N	ALA B		34.457	16.971	14.291	1.00 20.63	В
ATOM	2381	CA	ALA B		34.987	17.428	13,007	1.00 22.13	В
ATOM	2382	СВ	ALA B		35.571	16.236	12.244	1.00 20.20	В
ATOM	2383	c	ALA B		34.057	18.222	12.078	1.00 22.42	В
ATOM	2384	ō	ALA B		34.512	19.129	11.400	1.00 24.48	В
ATOM	2385	N	GLN B		32.772	17.893	12.036	1.00 25.59	В
ATOM	2386	CA	GLN B	126	31.845	18.598	11.147	1.00 27.46	В
ATOM	2387	CB	GLN B	126	30.414	18.101	11.357	1.00 29.99	В
ATOM	2388	CG	GLN B	126	30.283	16.595	11.480	1.00 36.21	В
ATOM	2389	CD	GLN B	126	30.625	16.102	12.870	1.00 38.28	В
MOTA	2390	OE1	GLN B	126	30.558	14.905	13.158	1.00 40.46	В
ATOM	2391	NE2	GLN B	126	30.989	17.030	13.745	1.00 40.92	В
ATOM	2392	C	GLN B		31.876	20.112	11.333	1.00 28.28	В
MOTA	2393	0	GLN B		31.571	20.627	12.410	1.00 29.36	В
ATOM	2394	N	ILE B		32.221	20.831	10.273	1.00 27.17	В
ATOM	2395	CA	ILE B		32.292	22.279	10.353	1.00 27.02	В
ATOM	2396	СВ	ILE B		33.656	22.716	10.931	1.00 27.21	B B
ATOM	2397		ILE B		34.767	22.453	9.898	1.00 21.63 1.00 24.63	В
ATOM	2398		ILE B ILE B		33.612	24.195 24.633	11.316 12.198	1.00 25.86	В
ATOM	2399 2400	CDI	IPE B		34.760 32.117	22.903	8.969	1.00 27.10	В
ATOM ATOM	2400	o	ILE B		32.393	22.258	7.956	1.00 26.58	В
ATOM	2401	N	LYS B		31.666	24.155	8.940	1.00 25.41	В
ATOM	2402	CA	LYS B		31.457	24.884	7.689	1.00 27.45	В
ATOM	2404	СВ	LYS B		29.964	24.927	7.334	1.00 29.68	В
ATOM	2405	CG	LYS B		29.633	25.685	6.046	1.00 34.69	В
ATOM	2406	CD	LYS B		30.129	24.954	4.793	1.00 38.25	В
ATOM	2407	CE	LYS B	128	29.802	25.742	3.517	1.00 40.20	В
ATOM	2408	NZ	LYS B	128	30.281	25.071	2.271	1.00 39.87	В
MOTA	2409	C	LYS B	128	31.983	26.301	7.861	1.00 25.41	В
MOTA	2410	0	LYS B		31.559	27.019	8.759	1.00 26.68	В
MOTA	2411	N	VAL B		32.911	26.700	7.002	1.00 25.70	В
MOTA	2412	CA	VAL B		33.493	28.034	7.078	1.00 24.82	В
MOTA	2413	CB	VAL B		35.013	27.956	7.329	1.00 24.17	В
ATOM	2414		VAL B		35.592	29.351	7.452	1.00 22.14	B B
ATOM	2415		VAL B		35.295	27.136	8.583	1.00 22.44	В
MOTA MOTA	2416	C	VAL B		33.248 33.532	28.791 28.283	5.778 4.701	1.00 25.17 1.00 25.50	В
ATOM	2417 2418	Ŋ	ARG B		32.724	30.007	5.884	1.00 27.21	В
MOTA	2419	CA	ARG B		32.445	30.814	4.701	1.00 28.49	В
ATOM	2420	CB	ARG B		30.931	30.920	4.470	1.00 31.77	В
ATOM	2421	CG	ARG B		30.239	29.591	4.183	1.00 34.92	В
ATOM	2422	CD	ARG B		28.927	29.813	3.432	1.00 41.30	В
ATOM	2423	NE	ARG B		27.834	30.254	4.291	1.00 42.15	В
MOTA	2424	CZ	ARG B		27.032	29.426	4.953	1.00 46.05	В
MOTA	2425	NHI	ARG B	130	27.200	28.112	4.849	1.00 45.50	В
MOTA	2426	NH	ARG B	130	26.061	29.910	5.718	1.00 48.30	В
ATOM	2427	C	ARG B	130	33.036	32.211	4.792	1.00 27.57	В
ATOM	2428	0	ARG B	130	33.130	32.789	5.874	1.00 26.00	В
ATOM	2429	N	TRP B		33.440	32.744	3.645	1.00 27.37	В
MOTA	2430	CA	TRP B		34.004	34.085	3.571	1.00 30.27	В
ATOM	2431	CB	TRP B		35.281	34.083	2.737	1.00 30.21	В
MOTA	2432	CG	TRP B		36.532	33.844	3.521	1.00 32.32	B
MOTA	2433		TRP B		37.155	34.757	4.432	1.00 32.41 1.00 33.07	В
ATOM	2434		TRP B		38.334 36.831	34.142 36.039	4.900 4.897	1.00 33.07	В
MOTA MOTA	2435		3 TRP B 1 TRP B		37.333	36.033	3.478	1.00 32.80	В
ATOM	2436 2437		1 TRP B		38.420	32.741	4.300	1.00 31.53	В
	243 (2423.	D						

MOTA	2438	CZ2	TRP B	131	39.193	34.764	5.812	1.00 32.82	В
MOTA	2439		TRP B		37.680	36.656	5.800	1.00 32.08	В
ATOM	2440		TRP B		38.849	36.017	6.249	1.00 33.40	В
ATOM	2441	C 0	TRP B		33.003	35.064	2.949	1.00 32.99	B B
MOTA MOTA	2442 2443	N	TRP B		32.367 32.879	34.759 36.242	1.940 3.550	1.00 32.18 1.00 35.48	В
MOTA	2444	CA	PHE B		31.962	37.263	3.058	1.00 39.35	В
MOTA	2445	СВ	PHE B		30.856	37.501	4.077	1.00 38.14	В
ATOM	2446	CG	PHE B		29.843	36.407	4.123	1.00 38.39	В
MOTA	2447	CD1	PHE B	132	28.804	36.373	3.202	1.00 38.31	В
MOTA	2448		PHE E		29.930	35.399	5.075	1.00 38.21	В
MOTA	2449		PHE E		27.860	35.348	3.229	1.00 39.26	В
ATOM	2450		PHE E		28.992	34.369	5.111	1.00 38.83 1.00 37.91	В
MOTA	2451	CZ	PHE P		27.954 32.650	34.345 38.583	4.184 2.755	1.00 37.91	B B
ATOM ATOM	2452 2453	o	PHB E		33.515	39.025	3.508	1.00 42.72	В
ATOM	2454	N	ARG E		32.267	39.203	1.640	1.00 45.04	В
ATOM	2455	CA	ARG E		32.829	40.490	1.242	1.00 48.28	В
ATOM	2456	CB	ARG E	133	32.510	40.787	-0.227	1.00 51.68	В
MOTA	2457	CG	ARG E		33.293	41.958	-0.829	1.00 55.78	В
MOTA	2458	CD	ARG E		34.787	41.655	-0.867	1.00 57.07	В
MOTA	2459	NE	ARG E		35.580	42.741	-1.440	1.00 59.30	В
MOTA	2460 2461	CZ	ARG E		35.523	43.135	-2.710 -3.564	1.00 60.93 1.00 61.44	B B
ATOM ATOM	2462		ARG E		34.702 36.295	42.536 44.132	-3.128	1.00 61.77	В
ATOM	2463	C	ARG E		32.129	41.492	2.145	1.00 49.07	В
ATOM	2464	ō	ARG E		32.299	41.460	3.358	1.00 51.26	В
ATOM	2465	N	ASN E		31.331	42.376	1.572	1.00 49.23	В
ATOM	2466	CA	ASN E	3 134	30.614	43.336	2.393	1.00 48.83	В
ATOM	2467	CB	asn i		30.582	44.702	1.710	1.00 45.93	В
MOTA	2468	CG	ASN E		31.973	45.290	1.523	1.00 45.10	В
ATOM	2469		ASN I		32.450	45.440	0.397	1.00 41.81	В
ATOM	2470 2471	C MD5	ASN E		32.634 29.203	45.618 42.795	2.634 2.594	1.00 41.82 1.00 50.25	B B
ATOM ATOM	2472	o	ASN I		28.222	43.529	2.508	1.00 52.28	В
ATOM	2473	N	ASP I		29.122	41.496	2.868	1.00 50.15	В
MOTA	2474	CA	ASP E		27.847	40.819	3.072	1.00 51.07	В
MOTA	2475	C	ASP E	3 135	27.590	39.855	1.910	1.00 51.76	В
MOTA	2476	0	ASP E		26.586	39.136	1.893	1.00 51.82	В
ATOM	2477	N	GLN E		28.507	39.856	0.944	1.00 50.97	В
MOTA	2478	CA	GLN I		28.421	38.999	-0.240	1.00 51.24	B B
MOTA MOTA	2479 2480	CB	GLN I	3 136 3 136	28.766 28.736	39.805 39.000	-1.493 -2.783	1.00 53.78 1.00 58.16	В
ATOM	2481	æ	GLN I		29.675	39.559	-3.839	1.00 59.39	В
MOTA	2482		GLN I		30.895	39.527	-3.675	1.00 60.12	В
MOTA	2483	NE2			29.110	40.078	-4.926	1.00 59.45	В
MOTA	2484	С		3 136	29.395	37.825	-0.124	1.00 49.46	В
MOTA	2485	0		3 136	30.607	38.026	-0.035	1.00 48.29	В
MOTA	2486	N		B 137	28.873	36.603	-0.144	1.00 47.64	В
ATOM	2487	CA CB		B 137 B 137	29.730 28.899	35.432 34.152	-0.027 0.022	1.00 46.85 1.00 47.17	B B
ATOM ATOM	2488 2489	CG		B 137	29.695	32.975	0.556	1.00 50.22	В
ATOM	2490		GLU I		28.866	31.726	0.743	1.00 52.65	В
ATOM	2491		GLU 1		27.699	31.842	1.171	1.00 55.57	В
MOTA	2492	OE2	GLU I	B 137	29.391	30.623	0.478	1.00 54.41	В
ATOM	2493	C		B 137	30.755	35.320	-1.149	1.00 45.23	В
MOTA	2494	0		B 137	30.445	35.544	-2.314	1.00 45.04	В
ATOM	2495	N		B 138 B 138	31.983 33.078	34.977	-0.776 -1.724	1.00 44.63 1.00 44.36	B B
ATOM ATOM	2496 2497	CA CB		B 138	34.284	34.808 35.658	-1.307	1.00 45.65	В
ATOM	2498	CG		B 138	34.076	37.166	-1.320	1.00 48.42	В
ATOM	2499	CD		B 138	34.144	37.761	-2.717	1.00 50.71	В
ATOM	2500		GLU :		35.120	37.471	-3.442	1.00 51.60	В
ATOM	2501	OE2	GLU :	B 138	33.227	38.526	-3.086	1.00 50.99	В
MOTA	2502	C		B 138	33.498	33.335	-1.740	1.00 43.68	В
ATOM	2503	0		B 138	33.831	32.769	-0.697	1.00 43.53	В
MOTA	2504	N		B 139	33.468 33.881	32.711 31.313	-2.914 -3.044	1.00 42.58 1.00 41.76	B B
MOTA MOTA	2505 2506	CA CB		В 139 В 139	32.739	30.415	-3.543	1.00 41.70	В
ATOM	2507		THR		32.207	30.948	-4.759	1.00 40.71	В
ATOM	2508		THR		31.641	30.325	-2.492	1.00 41.89	В
ATOM	2509	C	THR	B 139	35.038	31.245	-4.026	1.00 40.93	В
ATOM	2510	0		B 139	35.855	30.326	-3.981	1.00 40.04	В
MOTA	2511	N	ALA	В 140	35.096	32.224	-4.920	1.00 40.67	В

36.179 32.305 -5.887 1.00 41.22 MOTA 2512 CA ALA B 140 B MOTA 2513 CB ALA B 140 35.714 33.016 -7.158 1.00 41.13 В ATOM 2514 C ALA B 140 37.247 33.126 -5.177 1.00 41.09 -4.693 1.00 43.11 В MOTA ALA B 140 36.976 34.232 2515 0 32.582 -5.102 ATOM 2516 N **GLY B 141** 38.455 1.00 39.60 В ATOM 2517 CA **GLY B 141** 39.526 33.278 -4.418 1.00 35.11 **GLY B 141** 39.739 32.651 -3.051 1.00 33.42 ATOM 2518 C -2.287 GLY B 141 40.605 33.076 1.00 31.24 В ATOM 2519 O 1.00 31.89 -2.750 MOTA 2520 N VAL B 142 38.945 31.628 В ATOM 2521 CA VAL B 142 39.033 30.937 -1.470 1.00 32.27 В VAL B 142 37.645 30.790 -0.813 1.00 31.90 ATOM 2522 CB 0.400 1.00 32.37 В CG1 VAL B 142 37.733 29.861 ATOM 2523 MOTA 2524 CG2 VAL B 142 37.125 32.161 -0.402 1.00 32.53 В 39.652 29.552 -1.564 1.00 31.26 R MOTA 2525 C VAL B 142 ATOM 2526 VAL B 142 39.211 28.712 -2.343 1.00 32.44 В 0 40.676 29.326 -0.752 1.00 30.76 В MOTA 2527 N VAL B 143 VAL B 143 41.357 28.045 -0.702 1.00 29.79 В MOTA 2528 CA 42.815 28.154 -1.162 1.00 29.63 В ATOM 2529 CB VAL B 143 2530 CG1 VAL B 143 43.439 26.768 -1.212 1.00 31.60 ATOM -2.514 1.00 33.43 42.885 28.819 В ATOM 2531 CG2 VAL B 143 VAL B 143 41.357 27.575 0.749 1.00 30.61 B MOTA 2532 C 1.667 1.00 28.64 MOTA 2533 ٥ VAL B 143 41.665 28.338 В 41.017 0.950 1.00 29.65 В **SER B 144** 26.313 ATOM 2534 N 40.970 25.756 2,282 1.00 28,42 В ATOM 2535 CA SER B 144 39.541 25.325 2.605 1.00 29.23 В MOTA 2536 CB SER B 144 1.00 33.81 В SER B 144 39.457 24.705 3.875 MOTA 2537 OG **SER B 144** 41.900 24.562 2.373 1.00 27.32 ATOM 2538 C 1.397 1.00 27.40 В 42.101 MOTA 2539 **SER B 144** 23.840 0 THR B 145 42.492 24.372 3.542 1.00 25.70 В ATOM 2540 N 3.755 1.00 24.82 CA THR B 145 43.364 23.227 В ATOM 2541 4.995 1.00 25.01 В THR B 145 44.272 23.418 ATOM 2542 CB 6.186 1.00 25.18 В MOTA 2543 OG1 THR B 145 43.467 23.399 45.022 24.743 4.923 1.00 23.27 В MOTA 2544 CG2 THR B 145 THR B 145 42.392 22.100 4.071 1.00 24.16 В MOTA 2545 C 4.272 1.00 23.86 41.200 22.335 MOTA 2546 0 THR B 145 4.081 1.00 23.17 В MOTA 2547 N PRO B 146 42.865 20.854 MOTA 2548 CD PRO B 146 44.116 20.231 3.618 1.00 22.29 R 1.00 23.18 В PRO B 146 41.854 19.852 4.419 MOTA 2549 CA 4.008 1.00 24.20 В 42.521 18.536 PRO B 146 MOTA 2550 CB 1.00 22.82 В MOTA 2551 CG PRO B 146 43.998 18.833 4.162 PRO B 146 41.597 19.945 5.933 1.00 22.63 В MOTA 2552 C 42.213 20.766 6.625 1.00 21.32 В PRO B 146 ATOM 2553 0 40.667 19.146 6.445 1.00 22.60 LEU B 147 MOTA 2554 N 1.00 22.34 В 40.414 7.883 ATOM 2555 CA LEU B 147 19.142 1.00 22.17 **LEU B 147** 39.241 18.216 8.213 В ATOM 2556 CB 38.934 17.973 1.00 24.53 В LEU B 147 9.691 ATOM CG 2557 38.629 19.288 10.368 1.00 25.95 В ATOM 2558 CD1 LRU B 147 1.00 25.55 37.746 17.026 9.826 В ATOM 2559 CD2 LEU B 147 C LEU B 147 41.710 18.609 8.515 1.00 21.99 В ATOM 2560 42.290 17.640 B.024 1.00 21.35 В ATOM **LEU B 147** 2561 0 42.175 19.246 9.581 1.00 20.48 В TLR B 148 ATOM 2562 N 10.228 1.00 19.15 В 43.406 18.813 MOTA 2563 CA ILE B 148 1.00 21.68 ILE B 148 44.392 19.990 10.403 B ATOM 2564 CB 11.065 1.00 20.10 В MOTA CG2 ILE B 148 45.666 19.505 2565 1.00 25.04 CG1 ILE B 148 44.728 20,609 9.041 В MOTA 2566 45.416 1.00 29.06 В ATOM 2567 CD1 ILE B 148 19.649 8.090 1.00 17.56 ILE B 148 43.160 18.208 11.603 В MOTA 2568 С ٥ ILE B 148 42.566 18.852 12.467 1.00 14.88 В MOTA 2569 43.625 16.973 11.795 1.00 15.95 ARG B 149 ATOM 2570 N 1.00 17.47 В CA ARG B 149 43.492 16.273 13.077 2571 ATOM 1.00 16.94 MOTA 2572 CB ARG B 149 43.420 14.763 12.852 В ARG B 149 43.202 13.941 14.128 1.00 20.29 R CG ATOM 2573 ARG B 149 43.252 12.448 13.821 1.00 21.64 В ATOM 2574 CD 1.00 21.97 42.168 12.028 12.938 ATOM 2575 NB ARG B 149 1.00 23.22 ATOM 2576 CZ ARG B 149 40.934 11.742 13.348 В 40.015 12.471 1.00 23.89 В NH1 ARG B 149 11.374 ATOM 2577 NH2 ARG B 149 40.623 14.636 1.00 23.11 11.803 MOTA 2578 1.00 17.66 16.603 13.937 ARG B 149 44.720 ATOM 2579 C 1.00 17.51 ARG B 149 45.850 16.311 13.549 В MOTA 2580 0 44.496 15.098 1.00 16.67 В ASN B 150 17.210 ATOM 2581 N 1.00 16.94 В ASN B 150 45.592 17.593 15.980 ATOM 2582 CA ASN B 150 16.890 1.00 15.38 ATOM 2583 CB 45.174 18.756 1.00 18.41 CG ASN B 150 16.118 44.899 20.034 ATOM 2584 15.249 1.00 19.05 ATOM 2585 OD1 ASN B 150 45.685 20.436

ATOM	2586	ND2	ASN B	150	43.790	20.691	16.440	1.00 17.88	В
MOTA	2587	C	ASN B		46.116	16.452	16.841	1.00 18.47	В
ATOM	2588	ō	ASN B		47.220	16.540	17.384	1.00 17.03	В
ATOM	2589	N	GLY B		45.324	15.391	16.968	1.00 17.77	В
ATOM	2590	CA	GLY B		45.734	14.251	17.770	1.00 19.16	В
MOTA	2591	C	GLY B		45.258	14.293	19.213	1.00 20.44	В
ATOM	2592	0	GLY B		45.198	13.264	19.877	1.00 22.31	В
ATOM	2593	N	ASP B		44.906	15.475	19.701	1.00 20.79	В
ATOM	2594	CA	ASP B		44.450	15.624	21.077	1.00 21.97	В
MOTA	2595	CB	ASP B		45.192	16.790	21.748	1.00 21.95	В
ATOM	2596	CG	ASP B		45.027	18.101	20.992	1.00 28.05	В
ATOM	2597		ASP B		45.764	19.060	21.300	1.00 30.94	В
ATOM	2598		ASP B		44.158	18.181	20.090	1.00 28.02	В
ATOM	2599	C	ASP B		42.939	15.847	21.175	1.00 20.51	В
ATOM	2600	o	ASP B		42,474	16.619	22.010	1.00 21.63	В
MOTA	2601	N	TRP B		42.183	15.166	20.322	1.00 19.19	В
ATOM	2602	CA	TRP B		40.724	15.278	20.300	1.00 16.82	В
ATOM	2603	СВ	TRP B		40.121	14.865	21.657	1.00 15.80	В
ATOM	2604	CG	TRP B		40.326	13.408	22.005	1.00 16.21	В
ATOM	2605		TRP B		39.415	12.322	21.756	1.00 16.58	В
ATOM	2606	CE2	TRP B		40.047	11.134	22.188	1.00 15.08	В
MOTA	2607	CE3	TRP B		38.125	12.238	21.211	1.00 15.69	В
MOTA	2608		TRP B		41.435	12.848	22.564	1.00 14.68	В
MOTA	2609		TRP B		41.278	11.483	22.677	1.00 15.53	В
ATOM	2610		TRP B		39.438	9.879	22.087	1.00 15.60	В
ATOM	2611	CZ3	TRP B		37.518	10.987	21.112	1.00 14.22	В
ATOM	2612	CH2			38.176	9.827	21.549	1.00 13.89	В
ATOM	2613	C	TRP B		40.194	16.660	19.890	1.00 16.09	В
ATOM	2614	ō	TRP B		39.159	17.110	20.379	1.00 14.28	В
ATOM	2615	N	THR B		40.929	17.342	19.020	1.00 15.11	В
ATOM	2616	CA	THR B		40.499	18.627	18.483	1.00 16.19	В
ATOM	2617	СВ	THR B		41.176	19.877	19.150	1.00 18.02	В
ATOM	2618		THR B		42.602	19.804	19.008	1.00 19.50	В
ATOM	2619		THR B		40.788	20.000	20.608	1.00 15.03	В
ATOM	2620	C	THR B		40.908	18.602	17.024	1.00 15.24	В
ATOM	2621	0	THR B		41.773	17.832	16.635	1.00 15.24	В
ATOM	2622	N	PHE B		40.269	19.437	16.220	1.00 18.04	В
ATOM	2623	CA	PHE B		40.577	19.538	14.801	1.00 16.03	В
ATOM	2624	CB	PHE B	155	39.404	19.042	13.938	1.00 16.98	В
ATOM	2625	CG	PHE B	155	39.069	17.579	14.118	1.00 17.58	В
MOTA	2626	CD1	PHE B	155	38.133	17.170	15.074	1.00 18.20	В
ATOM	2627	CD2	PHE B	155	39.670	16.611	13.312	1.00 17.71	В
MOTA	2628	CEL	PHE B	155	37.799	15.810	15.223	1.00 17.81	В
MOTA	2629	CE2	PHE B	155	39.346	15.250	13.451	1.00 17.57	В
MOTA	2630	CZ	PHE B	155	38.407	14.849	14.409	1.00 16.39	В
MOTA	2631	C	PHE B	155	40.793	21.015	14.503	1.00 16.67	В
MOTA	2632	0	PHE B	155	40.532	21.870	15.352	1.00 16.84	В
MOTA	2633	N	GLN E	156	41.281	21.312	13.304	1.00 14.72	В
MOTA	2634	CA	GLN B	156	41.467	22.689	12.886	1.00 14.66	В
MOTA	2635	CB	GLN E		42.811	23.264	13.357	1.00 16.69	В
MOTA	2636	CG	GLN B		44.039	22.698	12.669	1.00 15.65	В
MOTA	2637	СD	GLN E		45.292	23.486	13.011	1.00 17.87	В
MOTA	2638		GLN E		45.477	24.617	12.555	1.00 17.56	В
MOTA	2639		GLN B		46.153	22.897	13.830	1.00 15.40	В
ATOM	2640	C	GLN E		41.398	22.722	11.371	1.00 14.00	B
MOTA	2641	0	GLN E		41.477	21.691	10.716	1.00 15.17	В
MOTA	2642	N	ILE E		41.241	23.911	10.818	1.00 15.34	В
MOTA	2643	CA	ILE E		41.165	24.057	9.383	1.00 17.26	В
MOTA	2644	CB	ILE E		39.791	23.585	8.856	1.00 16.56	В
MOTA	2645		ILE E		38.675	24.429	9.474	1.00 13.07	В
MOTA	2646		ILE E		39.765	23.649	7.326	1.00 17.72	В
MOTA	2647		ILE E		38.583	22.913	6.712	1.00 14.50	В
MOTA	2648	C	ILE E		41.379	25.523	9.074	1.00 18.67	В
MOTA	2649	0	ILE E		40.823	26.391	9.745	1.00 22.28	В
MOTA	2650	N	LEU E		42.217	25.795	8.083	1.00 18.98	В
ATOM	2651	CA	LEU E		42.508	27.162	7.690	1.00 20.77 1.00 22,23	В
MOTA	2652	CB	LEU E		44.022	27.368	7.555	1.00 22.23	В
ATOM	2653	CG	TEO E		44.851	27.525	8.838	1.00 26.12	В
ATOM	2654		PEO E		44.689	26.320	9.740	1.00 29.01	B B
MOTA	2655		LEU E		46.311	27.701	8.465 6.371	1.00 28.45	В
ATOM	2656	C O	LEU I		41.817 41.934	27.484 26.734	5.401	1.00 19.39	В
ATOM ATOM	2657 2658	N	VAL I		41.934	28.596	6.346	1.00 21.67	В
ATOM	2659	CA	VAL I		40.380	29.011	5.141	1.00 21.90	В
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MOTA	2660	СВ	VAL B	159	38.855	29.061	5.365	1.00 22.06	В
ATOM	2661		VAL B		38.147	29.252	4.043	1.00 20.55	В
ATOM ATOM	2662 2663	CG2	VAL B VAL B		38.381 40.899	27.766 30.379	6.009 4.749	1.00 20.83 1.00 21.80	B B
ATOM	2664	ŏ	VAL B		40.721	31.357	5.473	1.00 20.82	В
MOTA	2665	N	MET B	160	41.555	30.416	3.592	1.00 23.56	В
ATOM	2666	CA	MET B		42.179	31.613	3.055	1.00 25.12	В
ATOM	2667	CB	MET B		43.580	31.257	2.559	1.00 26.80	В
MOTA MOTA	2668 2669	CG SD	MET B		44.479 45.850	30.736 29.700	3.678 3.145	1.00 32.00 1.00 38.02	B
ATOM	2670	CE	MET B		45.094	28.065	3.307	1.00 35.43	В
MOTA	2671	C	MET B		41.387	32.269	1.941	1.00 28.27	В
ATOM	2672	0	MET B		40.684	31.602	1.177	1.00 28.76	В
ATOM	2673	N	LEU B		41.518	33.588	1.854	1.00 29.59 1.00 32.69	B B
MOTA MOTA	2674 2675	CA CB	LEU B		40.820 39.669	34.366 35.142	0.845 1.487	1.00 32.89	В
ATOM	2676	CG	LEU B		39.031	36.199	0.586	1.00 31.56	В
MOTA	2677	CD1	LEU B	161	38.156	35.516	-0.460	1.00 29.64	В
ATOM	2678		LEU B		38.213	37.167	1.423	1.00 29.89	В
ATOM	2679	C O	LEU B		41.755 42.350	35.349 36.216	0.154 0.801	1.00 35.59 1.00 35.54	B B
ATOM ATOM	2680 2681	Ŋ	GLU B		41.895	35.213	-1.158	1.00 39.87	В
ATOM	2682	CA	GLU B		42.728	36.118	-1.927	1.00 44.05	В
MOTA	2683	CB	GLU B	162	42.995	35.565	-3.331	1.00 46.86	В
ATOM	2684	CG	GLU B		43.795	36.497	-4.239	1.00 50.98	В
ATOM	2685	CD	GLU B		45.274	36.537 36.802	-3.891 -2.715	1.00 54.75 1.00 56.53	B B
ATOM ATOM	2686 2687		GLU B		45.604 46.108	36.308	-4.796	1.00 55.16	В
ATOM	2688	C	GLU B		41.879	37.372	-2.029	1.00 44.69	В
ATOM	2689	0	GLU B	162	40.719	37.302	-2.434	1.00 44.39	В
ATOM	2690	N	MET B		42.436	38.514	-1.648	1.00 46.67	В
MOTA	2691	CA CB	MET B		41.670 40.881	39.746 39.949	-1.716 -0.412	1.00 49.56 1.00 51.22	B B
MOTA MOTA	2692 2693	CG	MET B		41.652	39.675	0.876	1.00 51.58	В
ATOM	2694	SD		163	42.910	40.901	1.274	1.00 56.87	В
MOTA	2695	CE	MET B	163	41.915	42.187	2.029-	1.00 54.89	В
ATOM	2696	C	MET B		42.487	40.986	-2.028	1.00 51.43	В
ATOM	2697 2698	N O	MET B		43.717 41.777	40.988 42.038	-1.942 -2.412	1.00 51.02 1.00 53.70	B B
ATOM ATOM	2699	CA	THR B		42.385	43.316	-2.738	1.00 56.61	В
ATOM	2700	CB	THR B		41.889	43.820	-4.116	1.00 57.48	В
MOTA	2701	OG1			40.457	43.744	-4.172	1.00 57.81	В
MOTA	2702	CG2			42.480	42.967	-5.234 -1.642	1.00 57.23 1.00 57.80	B B
MOTA MOTA	2703 2704	0	THR E		42.012 40.866	44.318 44.766	-1.555	1.00 57.08	В
ATOM	2705	N	PRO B		42.976	44.658	-0.770	1.00 58.98	В
ATOM	2706	CD	PRO E	165	44.315	44.055	-0.647	1.00 59.54	В
MOTA	2707	CA	PRO E		42.734	45.605	0.322	1.00 60.52	В
MOTA	2708	CB	PRO E		44.063 44.604	45.608 44.236	1.078 0.822	1.00 60.33 1.00 60.42	B B
MOTA MOTA	2709 2710	C	PRO E		42.347	47.002	-0.163	1.00 61.65	В
ATOM	2711	ō	PRO E		43.149	47.698	-0.790	1.00 61.24	В
MOTA	2712	N	GLN E		41.110	47.395	0.126	1.00 62.45	В
ATOM	2713	CA	GLN E		40.598	48.709	-0.250 -1.410	1.00 63.32 1.00 65.46	B B
ATOM ATOM	2714 2715	CB	GLN E		39.605 40.177	48.590 47.945	-2.661	1.00 69.00	В
ATOM	2716	CD	GLN I		39.195	47.942	-3.819	1.00 71.19	В
MOTA	2717	OE1	GLN E		38.071	47.448	-3.697	1.00 72.48	В
ATOM	2718	NE2			39.617	48.492	-4.954	1.00 72.65 1.00 62.65	В
MOTA	2719	C O	GLN I		39.893 39.021	49.287 48.635	0.970 1.550	1.00 62.65	B
MOTA MOTA	2720 2721	N	ARG I		40.266	50.501	1.366	1.00 61.62	. B
ATOM	2722	CA	ARG I		39.645	51.111	2.535	1.00 60.86	В
ATOM	2723	CB	ARG I		40.190	52.525	2.777	1.00 62.57	В
ATOM	2724	CG	ARG I		39.953	53.029	4.204	1.00 64.82 1.00 67.31	B B
MOTA MOTA	2725 2726	CD	ARG I	B 167 B 167	40.742	52.198 52.143	5.227 6.539	1.00 67.31	В
ATOM	2727	CZ		B 167	40.570	51.477	7.591	1.00 69.14	В
MOTA	2728	NH1	ARG	B 167	41.710	50.804	7.499	1.00 69.34	В
MOTA	2729		ARG 1		39.897	51.471	8.735	1.00 69.52	В
MOTA	2730	0		B 167 B 167	38.136 37.647	51.154 51.615	2.333 1.303	1.00 59.19 1.00 58.60	B B
ATOM ATOM	2731 2732	N		B 168	37.404	50.656	3.320	1.00 58.18	В
ATOM	2733	CA		B 168	35.959	50.632	3.226	1.00 56.57	В

ATOM	2734	С	GLY B	168	35.466	49.200	3.191	1.00 55.42	В
ATOM	2735	0	GLY B	168	34.306	48.924	3.495	1.00 55.98	В
MOTA	2736	N	ASP B	169	36.350	48.280	2.814	1.00 53.44	В
ATOM	2737	CA	ASP B	169	35.979	46.871	2.757	1.00 51.76	В
ATOM	2738	CB	ASP B	169	36.841	46.115	1.740	1.00 50.49	В
ATOM	2739	CG	ASP B		36.428	46.392	0.311	1.00 50.57	В
ATOM	2740		ASP B	169	35.207	46.479	0.060	1.00 49.92	В
ATOM	2741		ASP B		37.31B	46.507	-0.559	1.00 49.84	В
ATOM	2742	c	ASP B		36.083	46.181	4.110	1.00 49.36	В
ATOM	2743	ō	ASP B		37.066	46.343	4.836	1.00 48.92	В
MOTA	2744	N	VAL B		35.047	45.418	4.436	1.00 47.48	В
ATOM	2745	CA	VAL B		34.981	44.667	5.680	1.00 45.10	В
ATOM	2746	CB	VAL B		33.800	45.130	6.543	1.00 45.86	В
ATOM	2747		VAL B		33.702	44.268	7.795	1.00 46.26	В
ATOM			VAL B		33.702	46.598	6.906	1.00 46.23	В
	2748							1.00 43.62	В
ATOM	2749	C	VAL B		34.787	43.191	5.342		В
ATOM	2750	0	VAL B		33.774	42.807	4.762	1.00 42.86	
MOTA	2751	N	TYR B		35.762	42.367	5.704	1.00 41.69	В
ATOM	2752	CA	TYR B		35.694	40.935	5.425	1.00 38.95	В
MOTA	2753	СВ	TYR B		37.044	40.455	4.899	1.00 37.52	В
ATOM	2754	CG	TYR B		37.405	41.031	3.553	1.00 38.12	В
MOTA	2755		TYR B		37.023	40.391	2.376	1.00 37.52	В
ATOM	2756		TYR B		37.342	40.923	1.131	1.00 38.06	В
MOTA	2757		TYR B		38.118	42.224	3.454	1.00 37.54	В
MOTA	2758	CE2	TYR B		38.442	42.767	2.216	1.00 38.45	В
ATOM	2759	\mathbf{cz}	TYR B		38.052	42.110	1.056	1.00 39.25	В
ATOM	2760	OH	TYR B		38.372	42.641	-0.172	1.00 38.84	В
MOTA	2761	C	TYR B		35.314	40.139	6.671	1.00 37.46	В
MOTA	2762	0	TYR B		35.791	40.428	7.773	1.00 34.85	В
ATOM	2763	N	THR B		34.452	39.140	6.501	1.00 35.06	В
MOTA	2764	CA	THR B		34.049	38.328	7.638	1.00 35.81	В
MOTA	2765	CB	THR B		32.589	38.622	8.064	1.00 38.37	В
MOTA	2766		THR B		31.688	38.177	7.043	1.00 42.02	В
MOTA	2767	CG2	THR B	172	32.390	40.119	8.292	1.00 39.83	В
MOTA	2768	С	THR B	172	34.182	36.830	7.406	1.00 33.71	В
MOTA	2769	0	THR B	172	33.953	36.335	6.300	1.00 32.99	В
ATOM	2770	N	CYS B	173	34.578	36.123	8.463	1.00 32.09	В
ATOM	2771	CA	CYS B	173	34.714	34.670	8.438	1.00 31.08	В
ATOM	2772	C	CYS B	173	33.497	34.183	9.200	1.00 30.92	В
MOTA	2773	0	CYS E	173	33.240	34.614	10.326	1.00 32.70	В
MOTA	2774	CB	CYS E	173	35.988	34.214	9.155	1.00 31.48	В
ATOM	2775	SG	CYS E	173	36.338	32.436	8.983	1.00 31.85	В
ATOM	2776	N	HIS E	174	32.748	33.288	8.578	1.00 30.26	В
MOTA	2777	CA	HIS E	174	31.524	32.754	9.152	1.00 29.72	В
MOTA	2778	CB	HIS E	174	30.401	32.977	8.128	1.00 30.80	В
ATOM	2779	CG	HIS E	174	29.030	32.625	8.615	1.00 32.90	В
MOTA	2780	CD2	HIS E	174	28,016	33.405	9.058	1.00 33.11	В
MOTA	2781	ND1	HIS E	174	28.551	31.332	8.621	1.00 34.85	В
ATOM	2782	CE1	HIS F	174	27.299	31.332	9.044	1.00 37.21	В
ATOM	2783	NE2	HIS E	174	26.950	32.577	9.316	1.00 34.95	В
ATOM	2784	С	HIS E	174	31.751	31.271	9.449	1.00 28.49	В
MOTA	2785	0	HIS E	174	32.080	30.494	8.554	1.00 27.69	В
ATOM	2786	N	VAL E		31.584	30.888	10.710	1.00 27.48	В
ATOM	2787	CA	VAL E	175	31.810	29.508	11.121	1.00 25.94	В
ATOM	2788	CB	VAL E		32.988	29.418	12.126	1.00 25.31	В
MOTA	2789		VAL E		33.147	27.982	12.629	1.00 21.10	В
ATOM	2790		VAL E		34.271	29,896	11.462	1.00 22.12	В
ATOM	2791	C	VAL E		30.606	28.821	11.748	1.00 26.58	В
ATOM	2792	ō	VAL I		30.004	29.328	12.694	1.00 27.01	В
ATOM	2793	N	GLU I		30.274	27.652	11.212	1.00 27.17	В
MOTA	2794	CA	GLU I		29.168	26.846	11.712	1.00 28.51	В
ATOM	2795	СВ	GLU I		28.166	26.573	10.588	1.00 32.35	В
ATOM	2796	CG	GLU I		27.454	27.827	10.082	1.00 38.87	В
ATOM	2797	69		3 176	26.776	27.616	8.735	1.00 42.45	В
ATOM	2798		GLU I		25.947	26.684	8.618	1.00 43.07	В
ATOM	2799		GLU 1		27.075	28.386	7.794	1.00 42.94	В
ATOM	2800	C		B 176	29.750	25.536	12.235	1.00 27.34	В
ATOM	2801	Ö		B 176	30.576	24.900	11.574	1.00 26.12	В
ATOM	2802	N		B 177	29.308	25.134	13.420	1.00 26.08	В
MOTA	2802	CA		B 177	29.800	23.921	14.049	1.00 26.30	В
MOTA	2804	CB		B 177	31.132	24.244	14.738	1.00 24.58	В
ATOM	2805	CG		B 177	31.759	23.076	15.422	1.00 22.32	В
MOTA	2806		HIS		32.646	22.156	14.977	1.00 21.05	В
MOTA	2807		HIS		31.437	22.711	16.710	1.00 21.01	В
AT OIL	2507	_,_,		··	/				_

					33 007	21.613	17.030	1.00 23.72	В
ATOM	2808		HIS B		32.097				В
MOTA	2809		HIS B		32.838	21.255	15.995	1.00 23.87	
MOTA	2810	C	HIS B	177	28.762	23.413	15.057	1.00 27.87	В
MOTA	2811	0	HIS B	177	28.059	24.205	15.672	1.00 29.54	В
MOTA	2812	N	PRO B	178	28.654	22.085	15.237	1.00 29.57	В
ATOM	2813	CD	PRO B	178	29.365	21.025	14.501	1.00 28.96	B
ATOM	2814	CA	PRO B		27.687	21.497	16.175	1.00 31.71	В
ATOM	2815	CB	PRO B		28.062	20.019	16.166	1.00 30.49	В
						19.810	14.769	1.00 30.01	В
MOTA	2816	CG	PRO B		28.503				В
MOTA	2817	C	PRO B		27.649	22.071	17.595	1.00 33.29	
ATOM	2818	0	PRO B	178	26.619	22.020	18.256	1.00 35.00	В
ATOM	2819	N	SER B	179	28.762	22.615	18.067	1.00 34.96	В
MOTA	2820	CA	SER B	179	28.813	23.168	19.418	1.00 36.85	В
ATOM	2821	CB	SER B	179	30.261	23.228	19.896	1.00 35.35	В
ATOM	2822	OG	SER B		31.023	24.053	19.034	1.00 35.14	В
					28.206	24.564	19.522	1.00 38.40	В
MOTA	2823	C	SER B					1.00 37.27	В
MOTA	2824	0	SER B		27.953	25.056	20.619		В
MOTA	2825	N	LEU B		27.971	25.192	18.377	1.00 40.10	
MOTA	2826	CA	LEU B	180	27.434	26.545	18.340	1.00 41.36	В
ATOM	2827	CB	LEU B	180	28.162	27.352	17.269	1.00 39.74	В
MOTA	2828	CG	LEU B	180	29.677	27.432	17.422	1.00 39.93	В
ATOM	2829		LEU B	180	30.286	28.013	16.157	1.00 39.41	В
MOTA	2830		LEU B		30.021	28.279	18.636	1.00 39.61	В
					25.944	26.633	18.078	1.00 43.85	В
ATOM	2831	C	LEU B					1.00 44.25	В
ATOM	2832	0	LEU B		25.449	26.125	17.072		
MOTA	2833	N	GLN B		25.230	27.289	18.984	1.00 47.20	В
ATOM	2834	CA	GLN B	181	23.794	27.475	18.814	1.00 49.93	В
ATOM	2835	CB	GLN B	181	23.158	27.956	20.121	1.00 52.00	B
ATOM	2836	CG	GLN B	181	23.873	29.134	20.758	1.00 56.40	В
ATOM	2837	CD	GLN B		23.263	29.538	22.084	1.00 59.03	В
	2838		GLN B		22.087	29.908	22.153	1.00 60.55	В
ATOM		NE2			24.059	29.468	23.149	1.00 58.44	В
MOTA	2839						17.715	1.00 49.23	В
MOTA	2840	C	GLN B		23.635	28.522		1.00 49.91	В
MOTA	2841	0	GLN B		22.712	28.465	16.906		
MOTA	2842	N	ser b	182	24.560	29.474	17.688	1.00 48.48	В
ATOM	2843	CA	SER B	182	24.555	30.523	16.679	1.00 47.89	В
MOTA	2844	CB	SER B	182	24.241	31.879	17.314	1.00 48.68	В
MOTA	2845	OG	SER B	182	25.211	32.223	18.286	1.00 50.58	В
MOTA	2846	C	SER B		25.938	30.550	16.038	1.00 45.93	В
	2847	ō	SER B		26.945	30.354	16.714	1.00 45.13	В
ATOM						30.783	14.721	1.00 45.12	В
ATOM	2848	N	PRO B		26.004			1.00 44.93	В
ATOM	2849	CD	PRO B		24.911	31.096	13.784		В
ATOM	2850	CA	PRO B		27.302	30.819	14.042	1.00 43.29	
MOTA	2851	CB	PRO B	183	26.923	31.070	12.581	1.00 43.70	В
ATOM	2852	CG	PRO B	183	25.642	31.833	12.688	1.00 44.70	В
ATOM	2853	C	PRO B	183	28.254	31.876	14.593	1.00 40.67	В
MOTA	2854	o	PRO B		27.828	32.851	15.209	1.00 40.46	В
	2855	N	ILE B		29.547	31.664	14.382	1.00 37.76	В
MOTA			ILE B		30.550	32.607	14.842	1.00 35.88	В
MOTA	2856	CA				31.889	15.468	1.00 35.92	В
MOTA	2857	CB	ILE B		31.759			1.00 35.57	В
ATOM	2858		2 ILE B		32.907	32.867	15.657		В
MOTA	2859		1 ILE E		31,362	31.270	16.806	1.00 36.74	
MOTA	2860	CD	1 ILE E	184	32.475	30.477	17.458	1.00 36.59	В
MOTA	2861	C	ILE E	184	31.040	33.453	13.680	1.00 34.88	В
MOTA	2862	0	ILE E	3 184	31.412	32.932	12.630	1.00 35.06	В
MOTA	2863	N	THR E		31.043	34.764	13.876	1.00 34.50	В
		CA			31.500	35.675	12.845	1.00 34.32	В
MOTA	2864					36.592	12.341	1.00 35.40	В
MOTA	2865	CB			30.356			1.00 37.01	В
ATOM	2866		1 THR E		29.770	37.285	13.450		
MOTA	2867	CG	2 THR E	3 185	29.286	35.774	11.631	1.00 35.73	В
MOTA	2868	C	THR E	3 185	32.622	36.548			В
MOTA	2869	0	THR I	3 185	32.559	37.050			В
ATOM	2870		VAL I		33.652		12.560	1.00 32.69	В
ATOM	2871				34.791				В
	2872			B 186	36.041				В
MOTA			1 VAL I		37.212	_			В
ATOM	2873								В
MOTA	2874		2 VAL 1		35.766				В
MOTA	2875			B 186	35.023				
ATOM	2876	0	VAL	B 186	35.060				В
ATOM	2877	N	GLU 1	B 187	35.172				В
MOTA	2878			B 187	35.373			1.00 38.96	В
ATOM	2879			B 187	34.484		11.154	1.00 40.90	В
ATOM	2880			B 187	33.008				В
MOTA	2881			B 187	32.146				В
MION	2001				221,220				

ATOM	2882	OE1	GLU B	187	30.909	42.739	11.545	1.00 51.77	В
ATOM	2883	OE2	GLU B	187	32.701	43.997	11.363	1.00 49.79	В
ATOM	2884	C	GLU B	187	36.816	41.175	10.784	1.00 39.59	В
MOTA	2885	0	GLU B	187	37.637	40.998	11.684	1.00 39.84	В
ATOM	2886	N	TRP B	188	37.113	41.765	9.635	1.00 39.59	В
MOTA	2887	CA	TRP B	188	38.430	42.302	9.360	1.00 40.86	В
MOTA	2888	CB	TRP B	188	39.339	41.252	8.736	1.00 38.70	В
ATOM	2889	CG	TRP B	188	40.769	41.704	8.693	1.00 37.82	В
ATOM	2890	CD2	TRP B	188	41.421	42.383	7.615	1.00 36.62	В
ATOM	2891		TRP B		42.748	42.640	8.023	1.00 36.31	В
ATOM	2892	CE3	TRP B		41.013	42.799	6.340	1.00 36.14	В
ATOM	2893			188	41.698	41.583	9.686	1.00 37.31	В
ATOM	2894		TRP B		42.890	42.141	9.291	1.00 37.27	В
ATOM	2895	CZ2	TRP B		43.673	43.296	7.204	1.00 37.17	В
ATOM	2896	CZ3	TRP B		41.932	43.452	5.522	1.00 38.70	В
ATOM	2897	CH2	TRP B		43.249	43.694	5.960	1.00 37.13	В
ATOM	2898	C	TRP B		38.258	43.455	8.383	1.00 42.97	В
ATOM	2899	ō	TRP B		37.946	43.240	7.211	1.00 42.37	В
ATOM	2900	N	ARG B		38.442	44.678	8.864	1.00 46.69	В
ATOM	2901	CA	ARG B		38.303	45.842	7.999	1.00 50.32	В
	2902	CB	ARG B		37.731	47.040	8.776	1.00 52.18	В
MOTA		CG	ARG B		38.615	47.590	9.893	1.00 56.00	В
ATOM	2903		ARG B		38.234	47.041	11.270	1.00 59.95	В
ATOM	2904	CD	ARG B		38.639	45.650	11.479	1.00 63.62	В
ATOM	2905	NE			39.903	45.236	11.559	1.00 64.33	В
ATOM	2906	CZ	ARG B		40.899	46.105	11.447	1.00 65.45	В
ATOM	2907		ARG B		40.172	43.951	11.760	1.00 64.46	В
MOTA	2908	NH2				46.192	7.412	1.00 50.56	В
ATOM	2909	C	ARG B		39.664	46.119	8.100	1.00 50.34	В
ATOM	2910	0	ARG B		40.680		6.135	1.00 52.30	В
MOTA	2911	N	ALA B		39.684	46.554	5.476	1.00 54.16	В
ATOM	2912	CA	ALA B		40.933	46.911	3.987	1.00 55.33	В
MOTA	2913	CB	ALA B		40.846	46.592	5.679	1.00 55.33	В
MOTA	2914	C	ALA B		41.238	48.392		1.00 54.90	В
MOTA	2915	0	ALA B		40.300	49.147	6.023	1.00 56.19	В
MOTA	2916		ALA E		42.408	48.782	5.481		č
MOTA	2917	C	TEO C		32.073	1.033	33.225	1.00 35.70	c
MOTA	2918	0	LEU C		33.091	1.607	33.619	1.00 35.87	c
MOTA	2919	N	LEU C		29.791	1.906	32.702	1.00 36.17	
MOTA	2920	CA	LEU C		30.699	1.409	33.777	1.00 34.35	C
MOTA	2921	N	GITM C		32.105	0.072	32.307	1.00 34.64	C
MOTA	2922	CA	GLN C		33.374	-0.359	31.737	1.00 34.20	C
ATOM	2923	С	GTN C		33.250	-0.823	30.294	1.00 33.55	c
ATOM	2924	0	GTW (32.373	-1.610	29.955	1.00 33.68	
ATOM	2925	N	PRO C		34.130	-0.329	29.418	1.00 33.74	C
ATOM	2926	CD	PRO C		35.226	0.632	29.639	1.00 33.81	c
ATOM	2927	CA	PRO (34.064	-0.742	28.015	1.00 34.77	C
MOTA	2928	CB	PRO (35.027	0.222	27.329	1.00 34.33	C
MOTA	2929	CG	PRO (36.070	0.449	28.393	1.00 34.78	C
MOTA	2930	C	PRO (34.508	-2.195	27.890	1.00 34.42	C
MOTA	2931	0	PRO (2 3	35.435	-2.626	28.579	1.00 34.76	C
MOTA	2932	N	PHE (C 4	33.837	-2.947	27.024	1.00 31.97	C
MOTA	2933	CA	PHE (C 4	34.173	-4.355	26.812	1.00 32.26	C
MOTA	2934	CB	PHE (32.897	-5.193	26.632	1.00 34.22	c
ATOM	2935	CG	PHE (C 4	32.006	-5.235	27.852	1.00 37.02	c
MOTA	2936		1 PHE		32.481	-4.835	29.103	1.00 38.53	C
MOTA	2937	CD:	2 PHE (C 4	30.701	-5.726	27.756	1.00 40.29	C
MOTA	2938	CE	1 PHE (C 4	31.673	-4.925	30.248	1.00 40.80	C
MOTA	2939	CE	2 PHE	C 4	29.878	-5.824	28.891	1.00 41.19	C
MOTA	2940	CZ	PHE	C 4	30.369			1.00 40.74	C
MOTA	2941	C	PHE	C 4	35.052		25.571	1.00 29.17	C
ATOM	2942	0	PHE		34.655			1.00 30.93	c
ATOM	2943	N	PRO		36.257				C
MOTA	2944	CD	PRO	C 5	36.936				C
MOTA	2945	CA	PRO		37.168				C
MOTA	2946	CB	PRO		38.527				C
MOTA	2947	CG	PRO	C 5	38.335				C
MOTA	2948	C	PRO	C 5	37.043				C
MOTA	2949	0	PRO	C 5	36.403				C
MOTA	2950	N	GLN		37.666				C
ATOM	2951	CA			37.659				C
MOTA	2952	CE	GLN	C 6	37.506				C
MOTA	2953	CG	GLN	C 6	36.170				C
MOTA	2954				36.074				C
ATOM	2955	OE	I GLN	C 6	36.483	-7.760	17.773	1.00 23.94	С

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MOTA	2956		GLN		6	35.525	-5.766	18.149	1.00 20.70	С
MOTA	2957	С	GLN	С	6	38.996	-8.637	22.204	1.00 20.71	C
MOTA	2958	0	GLN	С	6	40.046	-8.008	22.105	1.00 19.85	C
ATOM	2959	N	PRO	C	7	38.974	-9.932	22.548	1.00 21.37	C
ATOM	2960	CD CD	PRO		7		-10.710	23.017	1.00 21.21	č
ATOM	2961	CA	PRO		7		-10.673	22.790	1.00 21.62	С
ATOM	2962	CB	PRO	C	7	39.783	-11.730	23.795	1.00 21.96	С
MOTA	2963	CG	PRO	C	7	38.416	-12.085	23.297	1.00 20.65	C
ATOM	2964	C	PRO		7		-11.316	21.511	1.00 24.05	Ċ
MOTA	2965	0	PRO		7		-11.577	20.588	1.00 22.84	C
MOTA	2966	N	GLU	C	8	42.051	-11.550	21.448	1.00 26.22	C
ATOM	2967	CA	GLU	С	8	42.631	-12.215	20.292	1.00 27.00	C
ATOM	2968	CB	GLU		8		-11.687	19.988	1.00 27.94	C
ATOM	2969	CG	GLU		8		-12.494	18.915	1.00 28.38	C
ATOM	2970	CD	GLU	С	8	44.043	-12.649	17.589	1.00 31.32	C
MOTA	2971	OE1	GLU	C	8	42.980	-13.309	17.564	1.00 31.69	С
ATOM	2972	OE2	GT U	C	8	44.514	-12.112	16.563	1.00 29.86	C
ATOM	2973	C	GLU		8		-13.691	20.676	1.00 28.48	C
MOTA	2974	0	GLU		8		-14.029	21.829	1.00 28.74	C
ATOM	2975	N	LEU	C	9	42.407	-14.571	19.721	1.00 30.08	C
MOTA	2976	CA	LEU	С	9	42.404	-15.998	20.002	1.00 31.21	C
ATOM	2977	СВ	LEU		9	41.313	-16.688	19.183	1.00 32.12	C
	2978				9		-16.072	19.302	1.00 33.78	Ċ
ATOM		CG.	LEU							
ATOM	2979		LEU		9		-16.866	18.457	1.00 35.00	C
ATOM	2980	CD2	LEU	C	9	39.481	-16.061	20.761	1.00 35.59	C
MOTA	2981	С	LEU	C	9	43.748	-16.641	19.712	1.00 31.83	С
ATOM	2982	ō	LEU		9		-16.415	18.658	1.00 30.94	C
									1.00 33.31	č
ATOM	2983	N	PRO		10		-17.442	20.657		
ATOM	2984	CD	PRO	С	10	43.774	-17.661	22.032	1.00 33.12	C
ATOM	2985	CA	PRO	С	10	45.545	-18.097	20.439	1.00 36.08	C
ATOM	2986	CB	PRO	C	10	45.926	-18.590	21.836	1.00 36.62	C
ATOM	2987	CG	PRO		10		-18.846	22.476	1.00 35.26	С
MOTA	2988	С	PRO		10		-19.229	19.430	1.00 37.51	C
ATOM	2989	0	PRO	С	10	44.495	-20.030	19.491	1.00 39.49	С
ATOM	2990	N	TYR	С	11	46.365	-19.269	18.488	1.00 38.68	C
ATOM	2991	CA	TYR	C	11	46.392	-20.305	17.463	1.00 40.24	C
	2992	c c	TYR		11		-20.782	17.290	1.00 42.03	c
MOTA										
ATOM	2993	0	TYR		11		-21.967	17.586	1.00 42.72	C
MOTA	2994	OXT	TYR	С	11	48.665	-19.949	16.870	1.00 42.75	C
ATOM	2995	СB	VAL	D	2	76.722	40.050	4.030	1.00 35.81	D
ATOM	2996		VAL		2	77.537	40.465	2.823	1.00 36.64	D
						76.313	38.577	3.893	1.00 37.71	ď
MOTA	2997		VAL		2					
ATOM	2998	С	VAL	D	2	76.622	40.298		1.00 31.61	D
ATOM	2999	0	VAL	D	2	75.696	39.494	6.653	1.00 31.96	D
ATOM	3000	N	VAL	D	2	78.625	39.207	5.418	1.00 32.12	D
ATOM	3001	CA	VAL		2	77.560	40.255	5.317	1.00 33.74	D
	3002						41.246	7.441	1.00 29.52	D
MOTA		N	ALA		3	76.864				
ATOM	3003	CA	ALA	D	3	76.053	41.379	8.653	1.00 27.92	D
MOTA	3004	CB	ALA	D	3	76.480	40.321	9.684	1.00 27.11	D
ATOM	3005	С	ALA	D	3	76.128	42.767	9.286	1.00 25.71	D
ATOM	3006	0	ALA		3	77.050	43.540	9.016	1.00 23.11	D
		N	ASP		4	75.152	43.070	10.137	1.00 24.26	D
MOTA	3007									
ATOM	3008	CA	ASP		4	75.109	44.354	10.825	1.00 24.77	D
MOTA	3009	CB	ASP	D	4	73.774	44.533	11.555	1.00 25.88	D
MOTA	3010	CG	ASP	D	4	72.595	44.668	10.611	1.00 26.24	D
ATOM	3011		ASP		4	71.449		11.080	1.00 24.74	D
MOTA	3012		ASP		4	72.811		9.416	1.00 28.25	D
MOTA	3013	C	ASP		4	76.230		11.857	1.00 25.96	D
MOTA	3014	0	asp	D	4	76.882	45.437	12.027	1.00 26.40	D
MOTA	3015	N	HIS	D	5	76.440	43.290	12.549	1.00 24.52	D
MOTA	3016	CA	HIS		5	77.469	43.204	13.582	1.00 24.25	D
ATOM	3017	СВ	HIS		5	76.836		14.972	1.00 23.42	D
MOTA	3018	CG	HIS		5	76.138		15.231	1.00 26.12	D
MOTA	3019	CD2	HIS	D	5	76.567		15.126	1.00 26.16	D
MOTA	3020	ND1	. HIS	D	5	74.830	44.667	15.657	1.00 25.67	D
MOTA	3021		HIS		5	74.481		15.799	1.00 26.53	D
MOTA	3022		HIS		5	75.516		15.484	1.00 25.96	D
								13.492	1.00 22.88	D
ATOM	3023	C	HIS		5	78.241				
MOTA	3024	0	HIS		5	77.657		13.258	1.00 22.31	D
ATOM	3025	N	VAL	, D	6	79.552	41.980	13.691	1.00 20.27	D
MOTA	3026	CA	VAI	ם	6	80.421	40.815	13.657	1.00 19.49	D
ATOM	3027	CB	VAI		6.	81.419		12.486	1.00 20.45	D
								12.564	1.00 19.85	Ď
ATOM ATOM	3028 3029		L VAI		6	82.357		11.161	1.00 15.85	D
			Z VAI	. 10	6	80.674	40.869	11.161	1.00 43.49	v

ATOM 3030 C VAL D 81.223 40.792 14.944 1.00 18.77 MOTA 3031 0 VAL D 6 81.767 41.812 15.352 1.00 17.70 3032 N ALA D 81.304 39,626 15.575 MOTA 7 1.00 18.23 ATOM 3033 CA ALA D 7 82.046 39.489 16.821 1.00 18.01 MOTA 3034 CB ALA D 81.080 39.452 18.006 1.00 17.61 MOTA 3035 C ALA D 82.899 38.239 16.838 1.00 17.37 ALA D 82.568 1.00 19.56 ATOM 3036 O 7 37.242 16.208 ATOM 3037 N SER D 8 84.008 38.306 17.562 1.00 17.07 84.892 ATOM 3038 CA SER D 37.158 17.712 1.00 15.46 СВ SER D 86.297 37.455 17.202 1.00 12.56 MOTA 3039 8 3040 OG SER D ATOM 8 86.324 37.492 15.789 1.00 18.97 ATOM 3041 C SER D 8 84.932 36.904 19.201 1.00 16.39 ATOM 3042 0 SER D 8 85.613 37.614 19.951 1.00 15.61 84.144 1.00 17.58 TYR D 35.930 19.637 ATOM 3043 N 9 21.044 1.00 18.51 ATOM 3044 CA TYR D 9 84.096 35.587 D TYR D 9 82.698 35.133 21.444 1.00 17.92 ATOM 3045 CB D CG TYR D 9 81.730 36.290 21.362 1.00 17.41 ATOM 3046 CD1 TYR D 82.056 37.523 21.928 1.00 16.27 ATOM 3047 9 ATOM 3048 CE1 TYR D 9 81.208 38.603 21.840 1.00 15.18 D ATOM 3049 CD2 TYR D 9 80.515 36.169 20.701 1.00 17.05 D MOTA 3050 CE2 TYR D 9 79.649 37.252 20.608 1.00 18.01 80,005 38.466 21.181 1.00 16.67 MOTA 3051 CZ TYR D 9 39.543 21.104 1.00 20.30 MOTA 3052 OH TYR D 9 79.157 9 85.120 34.508 21.115 1.00 19.92 ATOM 3053 С TYR D D TYR D 9 84.856 33.323 21.337 1.00 17.21 ATOM 3054 O 1.00 22.61 3055 N GLY D 10 86.321 34.989 20.843 MOTA 20.836 1.00 20.96 MOTA 3056 CA GLY D 10 87.478 34.160 GLY D 10 88.358 34.354 19.624 1.00 18.79 ATOM 3057 C 88.170 1.00 16.79 ATOM 3058 0 GLY D 10 33.693 18.618 VAL D 11 3059 N 89.275 35.307 19.683 1.00 17.75 MOTA 18.616 1.00 16.92 90.256 35.394 MOTA 3060 CA VAL D 11 3061 CB VAL D 11 90.666 36.829 18.242 1.00 17.76 MOTA 3062 CG1 VAL D 11 91.873 36.778 17.313 1.00 15.46 MOTA 3063 CG2 VAL D 11 89.522 37.544 17.544 1.00 13.00 MOTA 91.391 34.728 19.395 1.00 17.46 VAL D 11 MOTA 3064 C 35.266 20.405 1.00 18.93 MOTA 3065 O VAL D 11 91.865 D MOTA 3066 N ASN D 12 91.773 33.531 18.973 1.00 17.46 CA ASN D 12 92.831 32.779 3067 19.644 1.00 18.01 MOTA 3068 CB ASN D 12 1.00 16.68 31.360 19.969 D 92.339 MOTA 1.00 16.27 MOTA 3069 CG ASN D 12 91.179 31.356 20.955 D OD1 ASN D 12 91.346 30.989 22.115 1.00 14.97 MOTA 3070 ND2 ASN D 12 90.000 31.779 20.497 1.00 14.97 MOTA 3071 18.759 1.00 18.74 94.061 32.699 ATOM 3072 С ASN D 12 1.00 19.66 3073 ASN D 12 93.963 32.373 17.578 D ATOM 0 LEU D 13 95.221 32.969 19.344 1.00 20.75 D MOTA 3074 N LEU D 13 96.471 32.949 18.600 1.00 22.59 3075 CA ATOM 3076 CB LEU D 13 1.00 24.32 MOTA 96.841 34.387 18.234 3077 CG LEU D 13 98.215 34.672 17.632 1.00 25.29 ATOM 98.355 33.966 16.289 1.00 24.58 D ATOM 3078 CD1 LEU D 13 CD2 LEU D 13 98.380 36.177 17.475 1.00 23.52 ATOM 3079 19.330 LEU D 13 97.646 32,290 1.00 22.44 ATOM 3080 C 97.900 1.00 24.67 ATOM 3081 LEU D 13 32.578 20.494 0 98.350 31.397 18.641 1.00 23.69 D ATOM 3082 N TYR D 14 ATOM 3083 CA TYR D 14 99.535 30.740 19.196 1.00 25.57 99.223 19.765 1.00 26.53 29.360 ATOM 3084 СВ TYR D 14 1.00 28.87 MOTA 3085 CG TYR D 14 100.445 28.712 20.383 100.872 29.057 21.668 1.00 28.57 ATOM 3086 CD1 TYR D 14 MOTA 3087 CE1 TYR D 14 102.032 28.500 22.218 1.00 27.29 101.209 27.793 ..19,664 1.00 29.65 ATOM 3088 CD2 TYR D 14 1.00 26.94 D MOTA 102.369 27.235 20.204 3089 CE2 TYR D 14 ATOM 3090 CZ TYR D 14 102.773 27.592 21.477 1.00 27.22 D OH TYR D 14 103.914 27.039 22.008 1.00 29.69 ATOM 3091 100.553 30.574 18.074 1.00 26.73 ATOM TYR D 14 3092 C 100.210 1.00 27.22 30.128 16.980 ATOM 3093 0 TYR D 14 ATOM 3094 GLN D 15 101.800 30.945 18.338 1.00 26.92 D 102.847 30.820 17.332 1.00 27.70 MOTA 3095 CA GLN D 15 GLN D 15 103.164 32.179 16.710 1.00 27.39 ATOM 3096 CB 103.534 1.00 27.78 GLN D 15 17.704 ATOM 3097 CG 33,251 1.00 27.70 MOTA 3098 CD GLN D 15 103.806 34.590 17.044 103.723 35.638 17.685 1.00 31.07 MOTA 3099 OE1 GLN D 15 ATOM NE2 GLN D 15 104.142 34.562 15.763 1.00 25.83 3100 104.097 17.952 1.00 28.40 ATOM 3101 C GLN D 15 30.222 104.368 30.416 1.00 28.81 ATOM 19.141 3102 0 GLN D 15 ATOM 3103 N SER D 16 104.852 29.488 17.143 1.00 27.95

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ATOM	3104	CA	SER		16	106.070	28.834	17.611	1.00 28.04	D
MOTA	3105	CB	SER	D	16	106.613	27.887	16.534	1.00 25.04	D
MOTA	3106	OG	SER	D	16	106.879	28.581	15.330	1.00 26.28	D
ATOM	3107	C	SER	D	16	107.155	29.824	18.024	1.00 27.77	D
MOTA	3108	Ō	SER		16	107.922	29.558	18.946	1.00 26.81	D
ATOM		N	TYR		17	107.221	30.965	17.351	1.00 29.70	ם
	3109									
ATOM	3110	CA	TYR		17	108.228	31.953	17.694	1.00 32.41	D
ATOM	3111	CB	TYR	D	17	108.248	33.086	16.672	1.00 35.15	D
MOTA	3112	CG	TYR	D	17	109.440	33.986	16.864	1.00 40.80	D
MOTA	3113	CD1	TYR	D	17	110.719	33.556	16.508	1.00 43.28	D
ATOM	3114		TYR		17	111.836	34.345	16.743	1.00 44.62	D
ATOM	3115		TYR		17	109.308	35.235	17.460	1,00 40.97	D
							36.032		1.00 44.83	D
ATOM	3116	CB2	TYR		17	110.419		17.702		
MOTA	3117	CZ	TYR		17	111.679	35.580	17.341	1.00 45.74	D
ATOM	3118	OH	TYR	D	17	112.788	36.353	17.590	1.00 49.39	D
ATOM	3119	C	TYR	D	17	107.954	32.525	19.084	1.00 33.13	D
ATOM	3120	0	TYR	D	17	106.888	33.092	19.332	1.00 32.77	D
ATOM	3121	N	GLY		18	108.930	32.383	19.981	1.00 32.74	D
							32.867	21.341	1.00 31.76	D
ATOM	3122	CA	GLY		1.8	108.780				
ATOM	3123	С	GLY		18	108.958	31.716	22.311	1.00 32.63	D
ATOM	3124	0	GLY	Ð	18	110.005	31.600	22.948	1.00 34.20	D
ATOM	3125	N	PRO	D	19	107.946	30.840	22.452	1.00 33.13	D
ATOM	3126	CD	PRO	D	19	108.029	29.606	23.256	1.00 31.73	D
ATOM	3127	CA	PRO		19	106.663	30.906	21.741	1.00 32.71	D
		СВ	PRO		19	106.115	29.492	21.903	1.00 33.20	D
MOTA	3128								1.00 31.76	Ď
MOTA	3129	CG	PRO		19	106.591	29.128	23.280		
MOTA	3130	C	PRO	D	19	105.768	31.948	22.406	1.00 32.52	D
ATOM	3131	0	PRO	D	19	105.970	32.282	23.568	1.00 33.11	D
MOTA	3132	N	SER	D	20	104.786	32.463	21.676	1.00 31.92	D
ATOM	3133	CA	SER	D	20	103.886	33.455	22.246	1.00 30.99	D
ATOM	3134	CB	SER		20	104.287	34.867	21.795	1.00 30.92	D
		OG	SER		20	104.263	34.988	20.381	1.00 33.16	D
ATOM	3135									D
ATOM	3136	С	SER		20	102.441	33.172	21.852	1.00 30.01	
MOTA	3137	0	SER	D	20	102.179	32.428	20.902	1.00 29.42	D
ATOM	3138	N	GLY	D	21	101.512	33.763	22.598	1.00 27.60	D
MOTA	3139	CA	GLY	D	21	100.101	33.580	22.318	1.00 25.70	D
ATOM	3140	С	GLY		21	99.309	34.836	22.632	1.00 24.66	D
ATOM	3141	ō	GLY		21	99.848	35.798	23.187	1.00 23.84	D
						98.030	34.834	22.268	1.00 22.55	D
MOTA	3142	N	GLN		22					Ď
MOTA	3143	CA	GLN		22	97.149	35.974	22.527	1.00 20.16	
MOTA	3144	СВ	GLN	D	22	97.301	37.049	21.445	1.00 18.28	D
ATOM	3145	CG	GLN	D	22	96.416	38.284	21.672	1.00 18.60	D
MOTA	3146	CD	GLN	D	22	96.513	39.327	20.562	1.00 18.36	D
ATOM	3147	OR1	GLN	D	22	97.379	40.207	20.587	1.00 19.82	D
MOTA	3148		GLN		22	95.617	39.232	19.582	1.00 17.69	D
		C	GLN		22	95.699	35.517	22.561	1.00 18.61	D
MOTA	3149									Ď
MOTA	3150	0	GLN		22	95.301	34.638	21.790	1.00 17.26	
ATOM	3151	N	TYR		23	94.926	36.097	23.475	1.00 16.42	D
ATOM	3152	CA	TYR	D	23	93.507	35.785	23.592	1.00 16.21	D
MOTA	3153	CB	TYR	D	23	93.212	34.839	24.762	1.00 14.97	D
ATOM	3154	CG	TYR	D	23	91.750	34.438	24.798	1.00 14.24	D
ATOM	3155	CD1			23	91.309	33.318	24.109	1.00 14.49	D
	3156		TYR	_	23	89.969	33.004	24.029	1.00 14.23	D
ATOM						90.795	35.240	25.421	1.00 13.21	D
MOTA	3157		TYR		23					
MOTA	3158		TYR		23	89.443	34.934	25.344	1.00 13.08	D
ATOM	3159	CZ	TYP	D	23	89.039	33.814	24.647	1.00 12.88	Q
MOTA	3160	OH	TYP	Œ	23	87.710	33.471	24.566	1.00 16.44	D
ATOM	3161	C	TYF	D	23	92.751	37.089	23.806	1.00 15.56	D
MOTA	3162	o	TYF		23	93.014	37.817	24.763	1.00 16.57	D
ATOM	3163	N	THE		24	91.811	37.377	22.914	1.00 14.11	D
MOTA			THE		24	91.026	38.598	22.995	1.00 13.31	D
	3164	CA								D
MOTA	3165	CB	THE		24	91.606	39.692	22.071	1.00 16.07	
MOTA	3166		THE		24	91.682	39.176	20.734	1.00 17.94	D
MOTA	3167	CG2	THE	םו	24	92.992	40.116	22.514	1.00 13.19	D
ATOM	3168	C	THE	D	24	89.604	38.342	22.519	1.00 12.68	D
MOTA	3169	0	THE		24	89.306	37.287	21.994	1.00 15.13	D
ATOM	3170	N	HIS		25	88.726	39.312	22.727	1.00 13.47	D
ATOM	3171	CA	HIS		25	87.360	39.224	22.229	1.00 13.83	D
						86.326	39.132	23.346	1.00 11.26	D
ATOM	3172	CB	HIS		25				1.00 14.42	D
ATOM	3173	CG	HI		25	86.053	37.727	23.785		
ATOM	3174		2 HI		25	86.815	36.610	23.723	1.00 12.09	D
MOTA	3175	ND:	L HIS	S D	25	84.876	37.351	24.392	1.00 15.93	D
ATOM	3176	CE:	L HI	S D	25	84.922	36.064	24.685	1.00 14.24	D
MOTA	3177	NE:	2 HI	B D	25	86.089	35.591	24.289	1.00 13.67	Ø
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ATOM	3178	C	HIS	D	25	87.158	40.495	21.436	1.00 13.30	D
ATOM	3179	0	HIS	D	25	87.573	41.563	21.859	1.00 13.77	D
ATOM	3180	N	GLU	D	26	86.544	40.376	20.271	1.00 15.40	D
ATOM	3181	CA	GLU		26	86.318	41.540	19.434	1.00 16.53	D
ATOM										
	3182	CB	GLU		26	87.109	41.396	18.133	1.00 14.47	D
MOTA	3183	CG	GLU		26	88.627	41.460	18.277	1.00 14.81	D
ATOM	3184	CD	GLU		26	89.341	41.205	16.947	1.00 19.22	D
ATOM	3185	OE1	GΤΩ	D	26	88.726	41.429	15.884	1.00 22.84	D
MOTA	3186	QE2	GLU	D	26	90.512	40.792	16.953	1.00 17.41	D
ATOM	3187	C	GLU	D	26	84.841	41.721	19.111	1.00 17.28	D
ATOM	3188	ō	GLU		26	84.073	40.760	19.100	1.00 16.62	D
ATOM	3189	N	PHE		27				1.00 19.63	
						84.455	42.971	18.879		D
ATOM	3190	CA	PHE		27	83.092	43.313	18.494	1.00 19.71	D
ATOM	3191	CB	PHE		27	82.231	43.722	19.684	1.00 21.05	Ø
ATOM	3192	CG	PHB	D	27	80.758	43.816	19.348	1.00 24.29	D
ATOM	3193	CD1	PHE	D	27	79.971	42.668	19.278	1.00 23.22	D
ATOM	3194	CD2	PHE	D	27	80.169	45.047	19.073	1.00 22.47	D
ATOM	3195	CE1	PHE	D	27	78.617	42.744	18.940	1.00 24.89	D
ATOM	3196		PHE		27	78.818	45.132	18.733	1.00 24.72	D
MOTA	3197	CZ	PHE		27			18.667	1.00 22.80	
						78.041	43.980			D
ATOM	3198	C	PHE		27	83.182	44.482	17.532	1.00 18.41	D
ATOM	3199	0	PHE		27	83.700	45.545	17.879	1.00 19.21	D
ATOM	3200	N	ASP	D	28	82.680	44.272	16.321	1.00 18.46	D
ATOM	3201	CA	ASP	D	28	82.700	45.284	15.272	1.00 18.63	D
ATOM	3202	CB	ASP	D	28	81.702	46.404	15.568	1.00 19.29	D
ATOM	3203	CG	ASP		28	80.268	45.981	15.305	1.00 22.52	D
ATOM	3204		ASP		28	80.076	44.885	14.738	1.00 23.13	D
			ASP							
ATOM	3205				28	79.333	46.736	15.651	1.00 24.61	D
ATOM	3206	C	ASP		28	84.075	45.865	15.037	1.00 17.83	D
ATOM	3207	0	ASP		28	84.225	47.069	14.860	1.00 20.60	D
MOTA	3208	N	GLY	D	29	85.079	44.997	15.042	1.00 18.44	D
ATOM	3209	CA	GLY	Ð	29	86.439	45.431	14.788	1.00 19.49	D
ATOM	3210	C	GLY	D	29	87.218	46.011	15.949	1.00 18.93	D
ATOM	3211	0	GLY		29	88.382	46.359	15.784	1.00 19.51	D
ATOM	3212	N	ASP		30	86.595	46.122	17.117	1.00 17.91	D
ATOM		CA	ASP		30	87.279	46.667	18.288	1.00 17.21	D
	3213									
ATOM	3214	СВ	ASP		30	86.499	47.858	18.831	1.00 15.85	D
ATOM	3215	CG	ASP		30	86.594	49.060	17.924	1.00 18.96	D
ATOM	3216		ASP		30	87.731	49.515	17.668	1.00 18.56	D
ATOM	3217	OD2	ASP	D	30	85.541	49.544	17.466	1.00 19.00	D
ATOM	3218	C	ASP	D	30	87.491	45.629	19.389	1.00 17.20	ם
ATOM	3219	0	ASP		30	86.651	44.763	19.621	1.00 15.68	D
ATOM	3220	N	GLU		31	88.629	45.739	20.062	1.00 18.79	D
ATOM	3221	CA	GLU		31	89.015	44.829	21.131	1.00 17.52	D
			GLU				44.947			Ď
ATOM	3222	СВ			31	90.531		21.363	1.00 19.03	
MOTA	3223	CG	GLU		31	91.074	44.215	22.579	1.00 22.08	Ð
MOTA	3224	œ	GLU		31	92.596	44.254	22.653	1.00 25.29	D
MOTA	3225	OE1	GLU	D	31	93.198	45.159	22.041	1.00 26.54	D
MOTA	3226	QE2	GLU	D	31	93.193	43.387	23.331	1.00 25.19	D
MOTA	3227	С	GLU	D	31	88.248	45.109	22.421	1.00 17.80	D
MOTA	3228	0	GLU	מ	31	88.360	46.195	23.004	1.00 16.81	D
ATOM	3229	N	GLN		32	87.478	44.118	22.862	1.00 15.25	Ø
ATOM		CA	GLN		32	86.685	44.230	24.085	1.00 15.53	D
	3230									
MOTA	3231	CB	GLN		32	85.502	43.260	24.044	1.00 12.86	D
MOTA	3232	CG	GLW		32	84.391	43.680	23.101	1.00 13.72	D
MOTA	3233	CD	GLN	D	32	83.233	42.708	23.111	1.00 16.53	D
MOTA	3234	OE1	GFN	D	32	83.407	41.526	22.838	1.00 20.27	D
ATOM	3235	NE2	GLN	D	32	82.044	43.203	23.423	1.00 17.48	D
ATOM	3236	С	GLN		32	87.528	43.956	25.329	1.00 16.00	D
ATOM	3237	Õ	GLN		32	87.356	44.603	26.366	1.00 15.18	Œ
ATOM	3238	N	PHE		33	88.423	42.981	25.222	1.00 16.17	ā
										ā
MOTA	3239	CA	PHE		33	89.315	42.638	26.321	1.00 15.74	
MOTA	3240	CB	PHE		33	88.520	42.083	27.515	1.00 15.40	D
ATOM	3241	CG	PHE	D	33	87.969	40.693	27.307	1.00 15.83	D
ATOM	3242	CD1	PHE	D	33	88.781	39.572	27.480	1.00 16.23	D
ATOM	3243	CD2	PHE	D	33	86.625	40.503	26.977	1.00 17.27	D
ATOM	3244		PHE		33	88.262	38.282	27.332	1.00 15.79	Ø
MOTA	3245		PHB		33	86.088	39.218	26.827	1.00 15.20	. <u>D</u>
ATOM		CZ	PHR		33	86.909	38.108	27.006	1.00 17.77	D
	3246									
MOTA	3247	C	PHE		33	90.330	41.614	25.860	1.00 15.28	D
MOTA	3248	0	PHE		33	90.157	40.979	24.825	1.00 15.16	D
MOTA	3249	N	TYR		34	91.405	41.476	26.620	1.00 15.54	D
ATOM	3250	CA	TYR	D	34	92.414	40.480	26.314	1.00 16.00	D
MOTA	3251	CB	TYR	D	34	93.649	41.124	25.670	1.00 17.46	D

94.508 41.970 26.588 1.00 20.90 MOTA 3252 CG TYR D 34 95.488 41.390 27.391 1.00 21.91 MOTA 3253 CD1 TYR D 34 D 96.295 42.174 28.221 1.00 24.17 ATOM 3254 CR1 TYR D 34 94.351 26.638 CD2 TYR D 34 43.354 1.00 20.26 MOTA 3255 95.147 44.141 27.463 1.00 24.97 ATOM 3256 CE2 TYR D 34 ATOM 3257 CZ TYR D 96.117 43.546 28.251 1.00 23.87 34 96.904 44.326 29.065 1.00 26.29 MOTA 3258 OH TYR D 34 27.642 1.00 16.56 MOTA 3259 C TYR D 34 92.766 39.836 MOTA 3260 O TYR D 34 92.476 40.386 28.699 1.00 15.36 93.354 38.653 27.586 1.00 18.29 MOTA VAL D 35 3261 N 1.00 19.11 37.971 28.795 ATOM 3262 CA VAL D 35 93.768 ATOM 3263 CB VAL D 35 93.257 36.514 28.842 1.00 17.61 D MOTA CG1 VAL D 35 93.910 35.780 29.992 1.00 17.99 D 3264 CG2 VAL D 35 91.744 36.493 29.003 1.00 17.82 ATOM 3265 95.290 28.813 1.00 19.96 37.950 ATOM 3266 C VAL D 35 VAL D 35 95.914 37.492 27.866 1.00 17.73 D MOTA 3267 0 38.473 29.880 1.00 22.63 3268 N ASP D 36 95.883 ATOM 97.333 38.456 30.005 1.00 24.79 ASP D 36 MOTA 3269 CA 1.00 26.41 31.106 MOTA 3270 CB ASP D 36 97.795 39.409 31,131 1.00 30,12 D ATOM 3271 CG ASP D ,36 99.298 39.574 100.002 38.547 31.252 1.00 32.04 D MOTA 3272 OD1 ASP D 36 OD2 ASP D 36 99.776 40.726 31.028 1.00 32.20 ATOM 3273 1.00 25.23 97.650 37.011 30.389 MOTA 3274 C ASP D 36 31.502 1.00 25.21 3275 ASP D 36 97.349 36.575 D MOTA 0 98.236 36.272 29.455 1.00 23.64 D 3276 N LEU D 37 ATOM 1.00 25.25 98.549 34.870 29.676 MOTA CA LEU D 37 3277 98.992 34.232 28.355 1.00 21.08 MOTA 3278 CB LEU D 37 27.225 1.00 20.24 D 3279 ÇG LEU D 37 97.955 34.360 ATOM 37 98.568 33.934 25.899 1.00 17.23 D MOTA 3280 CD1 LEU D 27.541 1.00 19.11 3281 CD2 LEU D 37 96.730 33.516 ATOM 30.770 1.00 27.73 LEU D 37 99.590 34.626 ATOM 3282 C 33.682 31.554 1.00 27.92 D 3283 LEU D 37 99.464 MOTA 0 100.608 35.474 30.837 1.00 29.31 D MOTA 3284 N GLY D 38 3285 CA 101.629 35.292 31.851 1.00 30.44 D GLY D 38 MOTA 33.242 1.00 32.52 101.141 35.640 MOTA 3286 C GLY D 38 34.220 1.00 34.37 D MOTA 3287 0 GLY D 38 101.502 34.986 MOTA 3288 N ARG D 39 100.309 36.669 33.335 1.00 35.10 D 34.623 1.00 36.92 D ARG D 39 99.786 37.103 МОТА 3289 CA 99.693 38.632 34.653 1.00 39.96 D ARG D 39 ATOM 3290 CB 34.301 1.00 44.57 MOTA 3291 CG ARG D 39 101.011 39.318 101.006 40.798 34.667 1.00 49.71 CD ARG D 39 MOTA 3292 34.270 1.00 53.08 D 102.240 41.484 3293 ARG D 39 ATOM NE 34.698 1.00 55.33 103.460 41.164 ATOM 3294 CZ ARG D 39 1.00 56.98 D NH1 ARG D 39 103.635 40.158 35.546 ATOM 3295 104.512 41.859 34.282 1.00 56.80 D ATOM 3296 NH2 ARG D 39 1.00 35.86 98.429 36.476 34.924 ARG D 39 MOTA 3297 C 97.886 36.022 1.00 35.27 3298 ARG D 39 36.630 ATOM 0 1.00 34.51 D LYS D 40 97.893 35.757 33,944 MOTA 3299 N 96.602 35.095 34.090 1.00 33.49 D LYS D 40 3300 CA MOTA 35.088 1.00 34.77 D 96.714 33.939 CB LYS D 40 ATOM 3301 95.482 33.040 35.133 1.00 41.38 LYS D 40 ATOM 3302 CG 95.703 31.839 36.046 1.00 45.02 œ LYS D 40 ATOM 3303 1.00 46.54 D 40 94.443 31.001 36.185 MOTA 3304 CE LYS D 94.652 29.853 37.112 1.00 48.98 D ATOM 3305 NZ LYS D 40 1.00 30.95 D 95.511 36.064 34.542 LYS D 40 ATOM 3306 С 35.794 35.492 1.00 28.23 3307 LYS D 40 94.780 ATOM 0 33.858 1.00 30.54 D GLU D 41 95.401 37.197 MOTA 3308 N GLU D 41 94.384 38.175 34.210 1.00 30.41 D MOTA 3309 CA 94.980 39.302 35.078 1.00 34.10 D GLU D 41 MOTA 3310 CB 96.180 40.034 34.488 1.00 41.52 D ÇG GLU D 41 ATOM 3311 1.00 45.72 D MOTA 3312 CD GLU D 41 96.834 40.997 35.482 1.00 48.68 OE1 GLU D 41 97.826 41.665 35.108 n ATOM 3313 1.00 47.60 D 96.362 41.086 36.638 OB2 GLU D 41 MOTA 3314 1.00 28.03 38.766 33.014 93.651 ATOM 3315 С GLU D 41 1.00 25.49 ATOM 3316 0 GLU D 41 94.220 38.981 31.940 42 92.364 39.006 33.226 1.00 25.48 MOTA N THR D 3317 42 91.488 39.582 32.224 1.00 23.42 D THR D CA ATOM 3318 1.00 22.07 90.035 32.511 D 42 39.187 ATOM 3319 CB THR D 1.00 18.54 3320 OG1 THR D 42 89.927 37.761 32.468 MOTA 1.00 20.32 42 89.087 39.817 31.497 ATOM CG2 THR D 3321 1.00 22.29 42 D THR D 91.615 41.098 32.301 C A'TOM 3322 1.00 21.54 42 91.492 41.680 33.373 ATOM 3323 0 THR D 1.00 21.50 D VAL D 43 91.874 41.736 31,167 3324 N ATOM 92.004 43.183 31.136 1.00 19.88 ATOM 3325 CA VAL D 43

ATOM	3326	СВ	VAL	D	43	93.428	43.584	30.697	1.00 21.56	D
ATOM	3327		VAL		43	93.620	45.091	30.828	1.00 20.99	D
ATOM	3328		VAL		43	94.456	42.827	31.539	1.00 19.79	מ
MOTA	3329	С	VĄŁ	D	43	90.968	43.744	30.164	1.00 20.50	D
ATOM	3330	0	VAL	D	43	91.045	43.513	28.959	1.00 19.49	D
ATOM	3331	N	TRP		44	89.987	44.466	30.690	1.00 21.49	D
ATOM	3332	CA	TRP	D	44	88.946	45.028	29.836	1.00 22.88	D
MOTA	3333	CB	TRP		44	87.685	45.326	30.649	1.00 21.57 1.00 21.99	D D
ATOM	3334	CG	TRP		44	87.167	44.129 43.125	31.372 30.854	1.00 22.20	D
MOTA	3335		TRP		44 44	86.280 86.119	42.150	31.862	1.00 22.19	Ď
ATOM ATOM	3336 3337	CE2			44	85.611	42.951	29.634	1.00 20.96	D
MOTA	3338		TRP		44	87.492	43.736	32.633	1.00 23.17	D
MOTA	3339	NE1			44	86.868	42.548	32.937	1.00 23.70	D
ATOM	3340	CZ2	TRP		44	85.311	41.016	31.693	1.00 24.30	D
ATOM	3341	CZ3	TRP	D	44	84.807	41.824	29.461	1.00 22.81	D
MOTA	3342	CH2	TRP	D	44	84.666	40.870	30.487	1.00 24.05	D
MOTA	3343	С	TRP	D	44	89.425	46.291	29.143	1.00 23.92	D
MOTA	3344	0	TRP		44	90.081	47.131	29.759	1.00 24.50	D
MOTA	3345	N	CYS		45	89.098	46.417	27.859	1.00 24.24	D D
MOTA	3346	CA	CYS		45	89.498	47.580	27.069 25.672	1.00 26.23 1.00 25.96	D
ATOM	3347	CB	CYS		45	89.951	47.141 46.098	25.665	1.00 25.42	D
ATOM	3348	SG	CYS		45 45	91.422 88.377	48.608	26.950	1.00 27.07	D
ATOM ATOM	3349 3350	0	CYS		45	88.612	49.749	26.549	1.00 28.23	D
ATOM	3351	N	LEU		46	87.157	48.193	27.273	1.00 27.18	D
ATOM	3352	CA	LEU		46	86.002	49.087	27.232	1.00 28.16	D
MOTA	3353	СВ	LEU		46	84.907	48.525	26.320	1.00 27.82	D
ATOM	3354	CG	LEU	D	46	84.142	49.460	25.372	1.00 30.22	D
MOTA	3355	CD1	LEU	םו	46	82.792	48.827	25.040	1.00 29.72	D
MOTA	3356		FEC		46	83.928	50.827	25.994	1.00 31.10	D
ATOM	3357	C	LEU		46	85.504	49.138	28.675 29.216	1.00 28.73 1.00 28.92	D D
ATOM	3358	0	LEU		46	85.049 85.601	48.133 50.309	29.318	1.00 29.35	D
ATOM	3359 3360	N CD	PRO		47 47	86.116	51.554	28.717	1.00 28.33	D
MOTA MOTA	3361	CA	PRO		47	85.182	50.533	30.709	1.00 29.01	D
ATOM	3362	СВ	PRO		47	85.139	52.051	30.806	1.00 29.32	D
ATOM	3363	CG	PRO		47	86.307	52,447	29.929	1,00 30.61	D
ATOM	3364	С	PRO	D	47	83.879	49.875	31.169	1.00 28.51	D
MOTA	3365	0	PRO		47	83.867	49.151	32.163	1.00 28.22	D
MOTA	3366	N	VAI		48	82.784	50.126	30.458	1.00 28.05 1.00 27.41	D D
MOTA	3367	CA	VAI		48	81.492 80.406	49.545 49.918	30.826 29.810	1.00 27.41	D
MOTA	3368	CB	VAI VAI		48 48	79.955	51.345	30.027	1.00 30.25	D
ATOM ATOM	3369 3370		VA		48	80.949	49.744	28.398	1.00 26.11	D
ATOM	3371	C		L D	48	81.490	48.022	30.961	1.00 26.77	D
ATOM	3372	o		L D	48	80.622	47.462	31.627	1.00 27.43	D
MOTA	3373	N	LE	J D	49	82.449	47.353	30.332	1.00 25.75	D
MOTA	3374	CA	LE	J D		82.517	45.898	30.395	1.00 27.21	D
MOTA	3375	CB		U D		83.237	45.354	29.153	1.00 27.47	D D
MOTA	3376	CG		U D		82.405	44.886	27.944 27.578	1.00 29.74 1.00 29.28	D
ATOM	3377		LLE			81.361 83.329	45.898 44.627	26.753	1.00 29.72	D
MOTA MOTA	3378 3379	c c	LE	U D		83.185	45.374	31.674	1.00 27.86	D
MOTA	3380	ō		ם ס		83.246	44.163	31.900	1.00 25.45	D
ATOM	3381	N		G D		83.680	46.283	32.508	1.00 29.82	D
ATOM	3382	CA	AR	G D	50	84.319	45.892	33.768	1.00 32.18	Ð
MOTA	3383	CB	AR	G D		84.900	47.105	34.509	1.00 35.49	D
MOTA	3384	ÇG		g D		86.010	47.890		1.00 40.53	D D
MOTA	3385	CD		G D		86.524	48.968		1.00 42.89 1.00 46.26	ם ס
MOTA	3386			GE		87.297	50.017		1.00 46.43	D
ATOM	3387	CZ	AR 1 AR	GE		88.484 89.049			1.00 46.42	ū
ATOM	3388 3389		2 AR			89.100			1.00 43.78	D
MOTA MOTA	3390			GI		83.283			1.00 31.58	D
ATOM	3391			G I		83.631			1.00 31.56	D
ATOM	3392			N I		82.009				D
MOTA	3393			NI		80.942				D
ATOM	3394			N I		79.610				D D
MOTA	3395			NI		79.194				D
MOTA	3396		GI 1 GI	N I		77.888 76.835				D
ATOM ATOM	3397 3398		2 GI			77.951			1.00 34.55	D
ATOM	3399			N I		80.830			1.00 29.51	D
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ATOM	3400	0	GLN D	51	80.291	42.721	35.911	1.00 29.09	D
ATOM	3401	N	PHE D	52	81.342	42.899	33.935	1.00 28.19	D
ATOM	3402	CA	PHE D	52	81.300	41.468	33.676	1.00 26.27	D
ATOM	3403	CB	PHE D	52	81.218	41.188	32.178	1.00 25.00	D
ATOM	3404	CG	PHE D	52 52	80.030	41.801 41.569	31.513 31.999	1.00 23.07 1.00 22.75	D D
Mota Mota	3405 3406		PHE D	52 52	78.744 80.188	42.594	30.380	1.00 22.75	D
MOTA	3407		PHE D	52	77.627	42.122	31.364	1.00 21.26	D
ATOM	3408		PHE D	52	79.079	43.151	29.735	1.00 21.92	D
ATOM	3409	CZ	PHE D	52	77.799	42,913	30.231	1.00 21.69	D
ATOM	3410	C	PHE D	52	82.547	40.797	34.217	1.00 27.11	Œ
MOTA	3411	0	PHE D	52	83.477	41.461	34.669	1.00 27.64	D
MOTA	3412	N	ARG D	53	82.556	39.471	34.152	1.00 27.25	D
MOTA	3413	CA	ARG D	53	83.683	38.672	34.609	1.00 28.31	D
ATOM	3414	CB	ARG D	53	83.347	37.976	35.939 37.143	1.00 32.75 1.00 40.59	D D
MOTA MOTA	3415 3416	CD	ARG D	53 53	83.263 82.418	38.921 38.325	38.269	1.00 45.99	Ď
ATOM	3417	NE	ARG D	53	81.007	38.229	37.892	1.00 52.14	Ď
ATOM	3418	cz	ARG D	53	80.172	39.265	37.808	1.00 53.70	D
ATOM	3419	NH1		53	80.597	40.493	38.080	1.00 53.85	D
ATOM	3420	NH2	ARG D	53	78.910	39.071	37.440	1.00 54.61	Ø
ATOM	3421	C	ARG D	53	84.007	37.624	33.548	1.00 25.73	D
ATOM	3422	0	ARG D	53	83.120	37.103	32.875	1.00 23.84	D
MOTA	3423	N	PHE D	54	85.290	37.335	33.387	1.00 23.47	D
ATOM	3424	CA	PHE D	54	85.716	36.336	32.425	1.00 19.92	D D
ATOM	3425	CB	PHE D	54	86.159	36.980	31.113 30.007	1.00 15.46 1.00 17.29	D
MOTA	3426	CG	DHE D	54 54	86.346 85.249	35.994 35.506	29.303	1.00 17.23	D
ATOM ATOM	3427 3428		PHE D	54 54	87.615	35.503	29.701	1.00 15.07	D
ATOM	3429		PHE D	54	85.415	34.539	28.309	1.00 16.04	D
ATOM	3430	CE2		54	87.788	34.535	28.709	1.00 13.99	D
ATOM	3431	cz	PHE D	54	86.688	34.055	28.014	1.00 14.35	D
MOTA	3432	C	PHE D	54	86.879	35.598	33.055	1.00 18.63	D
MOTA	3433	0	PHE D	54	87.922	36.188	33.329	1.00 19.50	D
MOTA	3434	N	ASP D	55	86.676	34.312	33.309	1.00 19.05	D
MOTA	3435	CA	ASP D	55	87.689	33.466	33.921	1.00 19.33	D D
MOTA	3436	CB	ASP D	55 55	87.084 88.090	32.100 31.138	34.237 34.832	1.00 21.38 1.00 24.95	D
MOTA	3437 3438	CG	ASP D ASP D	55 55	89.264	31.528	35.021	1.00 27.01	D
ATOM ATOM	3439		ASP D	55	87.703	29.985	35.112	1.00 27.48	D
MOTA	3440	C	ASP D	55	88.863	33.323	32.955	1.00 19.84	D
ATOM	3441	0	ASP D	55	88.741	32.691	31.904	1.00 18.07	D
MOTA	3442	N	PRO D	56	90.024	33.909	33.311	1.00 19.36	a
ATOM	3443	CD	PRO D	56	90.285	34.584	34.593	1.00 16.09	D
ATOM	3444	CA	PRO D	56	91.240	33.867	32.486	1.00 18.34	D
ATOM	3445	CB	PRO D	56	92.228	34.729	33.278 34.692	1.00 19.78 1.00 18.66	ם מ
ATOM	3446	CG	PRO D	56 56	91.792 91.770	34.517 32.468	32.206	1.00 18.30	Đ
MOTA MOTA	3447 3448	0	PRO D	56 56	92.583	32.277	31.299	1.00 17.41	D
ATOM	3449	Ŋ	GLN D	57	91.304	31.489	32.977	1.00 18.31	D
ATOM	3450	CA	GLN D	57	91.744	30.114	32.781	1.00 18.39	D
MOTA	3451	CB	GLN D	57	91.314	29.233	33.963	1.00 19.94	D
ATOM	3452	CG	GLM D	57	91.738	27.773	33.856	1.00 18.50	D
MOTA	3453	CD	GLN D		93.252	27.603	33.765	1.00 23.86	D
MOTA	3454		L GLN D		94.000	28.110	34.612	1.00 23.68	D
MOTA	3455		2 GLN D		93.709	26.885	32.739 31.480	1.00 19.56 1.00 20.01	D D
MOTA	3456	0	GLN D		91.174 91.733	29.555 28.618	30.903	1.00 19.26	Ď
ATOM ATOM	3457 3458	N	PHE D		90.059	30.113	31.016	1.00 19.19	D
ATOM	3459	CA	PHE D		89.490	29.629	29.765	1.00 20.37	D
ATOM	3460	СВ	PHE D		88.178	30.347	29.427	1.00 18.69	D
MOTA	3461	CG	PHE D	58	87.587	29.912	28.114	1.00 20.67	D
ATOM	3462		1 PHE D		88.040	30.456	26.912	1.00 19.84	D
ATOM	3463		2 PHE D		86.640	28.891	28.070	1.00 19.87	D
ATOM	3464		1 PHE D		87.562	29.984	25.682	1.00 19.25	D
ATOM	3465		2 PHE D		86.156	28.411	26.844	1.00 20.67 1.00 19.50	D D
MOTA	3466		PHE D		86.623 90.508	28.961 29.892	25.652 28.659	1.00 19.50	D
MOTA MOTA	3467 3468		PHE D		90.745	29.049	27.790	1.00 20.36	D
ATOM	3469		ALA D		91.115	31.070	28.716	1.00 20.85	D
MOTA	3470				92.111	31.477	27.736	1.00 21.87	D
ATOM	3471		ALA D	59	92.458	32.959	27.937	1.00 20.20	D
ATOM	3472		ALA D		93.374	30.618	27.819	1.00 22.41	D
MOTA	3473	0	ALA I	59	93.877	30.151	26.796	1.00 22.54	D

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ATOM	3474	N	LEU		60	93.890	30.409	29.030	1.00 21.24	D
ATOM	3475	CA	FEA	D	60	95.101	29.601	29.188	1.00 22.31	D
MOTA	3476	CB	LEU	D	60	95.501	29.474	30.663	1.00 22.79	D
ATOM	3477	CG	LEU	D	60	96.063	30.698	31.393	1.00 25.87	D
ATOM	3478	CD1	LEU	D	60	96.455	30.303	32.805	1.00 28.75	D
ATOM	3479		PEA		60	97.270	31.223	30.670	1.00 28.42	D
ATOM	3480	c	LEU		60	94.891	28.207	28.617	1.00 21.85	D
						95.731	27.691	27.875	1.00 22.48	Ď
ATOM	3481	0	LEU		60					
MOTA	3482	Ŋ	THR		61	93.763	27.600	28.966	1.00 19.32	D
ATOM	3483	CA	THR	D	61	93.457	26.259	28.489	1.00 20.67	D
ATOM	3484	CB	THR	D	61	92.175	25.721	29.158	1.00 20.04	D
ATOM	3485	OG1	THR	D	61	92.419	25.539	30.558	1.00 23.09	D
ATOM	3486		THR		61	91.759	24.393	28.546	1.00 21.15	D
		C	THR		61	93.283	26.240	26.974	1.00 19.50	D
ATOM	3487								1.00 18.76	Ď
MOTA	3488	0	THR		61	93.805	25.363	26.288		
ATOM	3489	N	asn		62	92.565	27.229	26.456	1.00 19.66	D
ATOM	3490	CA	asn	D	62	92.310	27.300	25.032	1.00 19.00	D
ATOM	3491	CB	ASN	D	62	91.356	28.453	24.729	1.00 18.52	D
ATOM	3492	CG	ASN	D	62	90.262	28.052	23.760	1.00 20.31	D
ATOM	3493		ASN		62	89.726	26.942	23.833	1.00 19.27	D
			ASN		62	89.917	28.952	22.854	1.00 22.25	D
MOTA	3494									D
MOTA	3495	С	ASN		62	93.599	27.445	24.244	1.00 19.63	
MOTA	3496	0	ASN	D	62	93.774	26.788	23.221	1.00 21.16	D
MOTA	3497	Ŋ	ILE	D	63	94.509	28.290	24.724	1.00 19.68	D
ATOM	3498	CA	ILE	D	63	95.779	28.481	24.033	1.00 18.76	D
ATOM	3499	CB	ILE		63	96.587	29.660	24.645	1.00 18.72	D
ATOM	3500	CG2	ILB		63	97.946	29.780	23.966	1.00 17.99	D
			ILE		63	95.813	30.968	24.471	1.00 17.09	D
MOTA	3501								1.00 17.47	Ď
MOTA	3502		ILE		63	95.507	31.313	23.017		
ATOM	3503	C	ILE	D	63	96.613	27.195	24.094	1.00 18.86	D
MOTA	3504	0	ILE	D	63	97.354	26.885	23.164	1.00 20.67	D
MOTA	3505	N	ALA	ם	64	96.497	26.448	25.188	1.00 18.22	D
ATOM	3506	CA	ALA		64	97.244	25.193	25.316	1.00 20.33	D
MOTA	3507	CB	ALA		64	97.039	24.574	26.708	1.00 17.30	D
						96.756	24.232	24.233	1.00 21.38	D
MOTA	3508	C	ALA		64					
MOTA	3509	0	ALA		64	97.536	23.459	23.677	1.00 23.44	D
ATOM	3510	N	VAL	D	65	95.459	24.290	23.940	1.00 21.97	Ð
MOTA	3511	CA	VAL	D	65	94.872	23.444	22.910	1.00 22.59	D
MOTA	3512	CB	VAL	D	65	93.324	23.570	22.890	1.00 22.30	D
MOTA	3513		VAL		65	92.744	22.781	21.728	1.00 17.73	D
		CG2			65	92,747	23.053	24.204	1.00 19.10	D
MOTA	3514							21.541	1.00 23.65	ם
MOTA	3515	С	VAL		65	95.441	23.832			
MOTA	3516	0	VAL		65	95.783	22.961	20.746	1.00 23.24	D
MOTA	3517	N	LEU	D	66	95.552	25.133	21.271	1.00 25.03	D
MOTA	3518	CA	LEU	D	66	96.102	25.580	19.991	1.00 26.10	D
MOTA	3519	СВ	LEU	D	66	96.104	27.111	19.870	1.00 23.98	D
ATOM	3520	CG	LEU	D	66	94.826	27.953	19.969	1.00 25.20	D
	3521		LEU		66	95.030	29.233	19.169	1.00 21.70	D
MOTA			LEU				27.211	19.435	1.00 26.16	D
MOTA	3522				66	93.629			1.00 26.24	D
MOTA	3523	C	LEU		66	97.533	25.078	19.880		
ATOM	3524	0	LEU	D	66	97.971	24.667	18.816	1.00 27.10	D
ATOM	3525	N	LYS	D	67	98.262	25.131	20.989	1.00 27.93	D
MOTA	3526	CA	LYS	D	67	99.642	24.658	21.024	1.00 28.00	D
MOTA	3527	СВ	LYS	D	67	100.215	24.827	22.437	1.00 27.69	D
ATOM	3528	CG	LYS		67	101.633	24.316	22.625	1.00 28.46	D
		CD	LYS		67	102.086	24.504	24.069	1.00 30.94	D
ATOM	3529							24.356	1.00 32.95	D
MOTA	3530	CE	LYS		67	103.401	23.791			
MOTA	3531	NZ	LYS		67	104.517	24.279	23.503	1.00 35.64	D
MOTA	3532	C	LYS	D	67	99.642	23.182	20.629	1.00 27.56	D
ATOM	3533	0	LYS	D	67	100.414	22.759	19.767	1.00 27.65	D
MOTA	3534	N	HIS	D	68	98.761	22.405	21.254	1.00 27.05	D
ATOM	3535	CA	HIS		68	98.665	20.982	20.956	1.00 26.31	D
ATOM	3536	CB	HIS		68	97.600	20.324	21.844	1.00 27,74	D
		CG	HIS		68	97.356	18.879	21.531	1.00 31.20	D
MOTA	3537								1.00 31.26	D
MOTA	3538		HIS		68	97.801	17.748	22.130		
MOTA	3539		L HIS		68	96.582	18.466	20.465	1.00 32.71	D
MOTA	3540	CE:	l HIE	D	68	96.560			1.00 31.32	D
MOTA	3541	NE:	2 HIS	g g	68	97.292	16.686	21.421	1.00 31.58	D
ATOM	3542	С	HIS			98.341	20.757	19.483	1.00 25.27	D
ATOM	3543	ō	HIS			98.958			1.00 25.67	D
	3544	И	ASI			97.386				D
MOTA										D
MOTA	3545					96.986				D
MOTA	3546					95.706				
MOTA	3547	CG	ASI	N D	69	94.447	21.504	17.805	1.00 24.20	D
								71		

2	2542			_		04 501	20 536	18.562	1.00 26.69	D
ATOM	3548		ASN		69	94.521	20.536			
MOTA	3549		asn		69	93.283	21.994	17.381	1.00 21.03	D
MOTA	3550	С	asn	D	69	98.091	21.855	16.601	1.00 24.52	D
MOTA	3551	0	NZA	D	69	98.329	21.223	15.570	1.00 22.82	D
MOTA	3552	N	LEU	D	70	98.763	22.954	16.934	1.00 24.56	D
MOTA	3553	CA	TEA		70	99.831	23.459	16.078	1.00 26.89	D
MOTA	3554	СВ	PEA		70	100.478	24.707	16.690	1.00 23.85	D
										D
MOTA	3555	CG	LEU		70	101.619	25.306	15.857	1.00 22.71	
MOTA	3556	CD1	LEU	D	70	101.082	25.776	14.519	1.00 19.18	D
MOTA	3557	CD2	LEU	D	70	102.254	26.472	16.592	1.00 23.62	D
ATOM	3558	C	LEU	D	70	100.900	22.388	15.882	1.00 28.63	D
MOTA	3559	ō	LEU		70	101.413	22.210	14.780	1.00 27.56	D
		N	ASN		71	101.224	21.687	16.967	1.00 31.13	Ď
ATOM	3560							16.962	1.00 35.25	D
ATOM	3561	CA	ASN		71	102.238	20.637			
MOTA	3562	СВ	asn		71	102.393	20.052	18.370	1.00 35.30	D
ATOM	3563	CG	asn	D	71	103.149	20.978	19.307	1.00 38.03	D
ATOM	3564	OD1	ASN	D	71	103.197	20.751	20.518	1.00 40.05	D
MOTA	3565	ND2	ASN	D	71	103.752	22.026	18.748	1.00 38.78	D
ATOM	3566	C	ASN		71	101.931	19.521	15.975	1.00 36.85	D
			ASN		71	102.829	18.997	15.316	1.00 36.91	D
MOTA	3567	0							1.00 38.08	D
MOTA	3568	N	SER		72	100.660	19.157	15.876		
ATOM	3569	CA	SER	D	72	100.261	18.104	14.961	1.00 39.44	D
MOTA	3570	CB	SER	D	72	98.847	17.623	15.306	1.00 40.69	D
MOTA	3571	OG	SER	D	72	98.529	16.427	14.611	1.00 44.84	D
MOTA	3572	c	SER		72	100.320	18.614	13.520	1.00 39.55	D
					72	100.798	17.915	12.625	1.00 38.61	D
ATOM	3573	0	SER						1.00 40.64	Ď
MOTA	3574	N	TEO		73	99.846	19.839	13.305		
MOTA	3575	CA	TEO	D	73	99.844	20.443	11.974	1.00 42.19	D
MOTA	3576	CB	LEU	D	73	99.085	21.768	11.990	1.00 42.17	α
ATOM	3577	CG	LEU	D	73	97.608	21.700	11.608	1.00 43.12	D
ATOM	3578	CD1	LEU		73	96.891	20.664	12.443	1.00 44.19	D
ATOM	3579		LEU		73	96.988	23.072	11.801	1.00 44.59	D
			LEU		73	101.237	20.678	11.407	1.00 43.27	D
MOTA	3580	C							1.00 43.00	D
MOTA	3581	0	LEU		73	101.466	20.479	10.215		
MOTA	3582	N	ILE	D	74	102.162	21.116	12.253	1.00 44.60	Ð
ATOM	3583	CA	ILE	D	74	103.529	21.364	11.812	1.00 46.44	D
MOTA	3584	CB	ILE	D	74	104.431	21.770	13.000	1.00 46.31	D
ATOM	3585		ILE		74	105.893	21.792	12.571	1.00 46.14	D
	3586		ILE		74	103.996	23.140	13.529	1.00 45.97	D
MOTA						104.683	23.561	14.812	1.00 43.97	D
MOTA	3587		ILE		74				1.00 48.14	D
ATOM	3588	C	ILE		74	104.077	20.095	11.166		
MOTA	3589	0	ILE	D	74	104.724	20.147	10.119	1.00 48.28	D
MOTA	3590	N	LYS	D	75	103.800	18.957	11.795	1.00 49.68	D
ATOM	3591	CA	LYS	D	75	104.252	17.669	11.290	1.00 51.82	D
ATOM	3592	СВ	LYS		75	104.060	16.589	12.356	1.00 52.85	D
MOTA	3593	CG	LYS		75	104.856	16.839	13.621	1.00 54.78	D
			LYS		75	104.517	15.831	14.704	1.00 57.28	D
MOTA	3594	CD.						16.010	1.00 58.75	D
MOTA	3595	CE	LYS		75	105.222	16.170			
MOTA	3596	NZ	LYS	D	75	104.803	15.266	17.116	1.00 59.97	D
MOTA	3597	C	LYS	D	75	103.499	17.276	10.023	1.00 52.37	D
MOTA	3598	0	LYS	D	75	104.106	17.086	B.972	1.00 52.78	D
ATOM	3599	N	ARG	D	76	102.177	17.171	10.124	1.00 52.67	Q
ATOM	3600	CA	ARG		76	101.353	16.783	8.986	1.00 52.67	D
			ARG		76	99.911	16.546	9.439	1.00 53.54	D
MOTA	3601	CB						10.346	1.00 55.62	D
MOTA	3602	CG	ARG		76	99.764	15.339			
ATOM	3603	CD	ARC		76	98.310	15.011	10.639	1.00 58.29	D
ATOM	3604	NB	ARC	3 D	76	97.628	16.107	11.319	1.00 61.07	D
MOTA	3605	CZ	ARC	Ð	76	96.437	16.000	11.900	1.00 62.21	D
ATOM	3606	NH:	1 ARC	a D	76	95.793	14.840	11.885	1.00 62.71	D
ATOM	3607		2 ARC		76	95.889	17.055	12.492	1.00 61.94	D
				3 D	76	101.375	17.761	7.816	1.00 52.35	D
MOTA	3608							6.817	1.00 52.65	מ
ATOM	3609			3 D	76	100.691	17.550		1.00 52.02	D
MOTA	3610	N		R D	77	102.160	18.824	7.932		
MOTA	3611	CA	SEI	R D	77	102.255	19.807	6.856	1.00 51.87	D
ATOM	3612	CB	SE	R D	77	101.945	21,212	7.379	1.00 50.95	D
ATOM	3613			R D		102.975	21.668	8.239	1.00 48.11	D
MOTA	3614			R D		103.667	19.789	6.287	1.00 52.25	D
				R D		104.028	20.633		1.00 51.67	D
MOTA	3615						18.814		1.00 52.79	D
MOTA	3616			N D		104.455			1.00 53.67	D
MOTA	3617			N D		105.841				
MOTA	3618			N D		105.912				D
MOTA	3619			N D		107.298				D
ATOM	3620	OD	1 AS	N D	78	107.959	17.129			D
MOTA	3621		2 AS			107.732		3.184	1.00 58.05	D

ATOM	3622	C	ASN	ъ	78	106.549	19.985	6.632	1.00 52.90	_
										D
ATOM	3623	0	asn		78	107.300	20.536	5.826	1.00 53.98	D
MOTA	3624	N	SER	D	79	106.275	20.479	7.835	1.00 51.25	D.
MOTA	3625	CA	SER	D	79	106.856	21.715	8.341	1.00 49.59	D
MOTA	3626	CB	SER	D	79	108.333	21.498	8.664	1.00 49.69	D
ATOM	3627	OG	SER	D	79	108.472	20.604	9.753	1.00 52.23	D
ATOM	3628	C	SER	D	79	106.711	22.931	7.437	1.00 47.21	D
ATOM	3629	ō	SER		79	107.699	23.588	7.111	1.00 47.49	D
	3630	N	THR		80	105.483	23.235	7.032	1.00 44.68	D
MOTA										
MOTA	3631	CA	THR		80	105.245	24.401	6.189	1.00 43.69	D
MOTA	3632	CB	THR		80	103.928	24.274	5.407	1.00 45.12	D
MOTA	3633	OG1	THR	D	80	103.976	23.112	4.570	1.00 47.94	D
MOTA	3634	CG2	THR	D	80	103.706	25.505	4.541	1.00 44.11	D
ATOM	3635	С	THR	D	80	105.166	25.634	7.094	1.00 42.94	D
ATOM	3636	0	THR		80	104.225	25.783	7.874	1.00 41.60	D
ATOM	3637	N	ALA		81	106.162	26.510	6.988	1.00 40.39	D
ATOM	3638	CA	ALA		81	106.215	27.715	7.804	1.00 37.86	D
										D
MOTA	3639	CB	ALA		81	107.657	28.171	7.958	1.00 39.23	
MOTA	3640	С	ALA		81	105.372	28.846	7.234	1.00 36.29	D
ATOM	3641	0	ALA	D	81	104.988	28.829	6.065	1.00 35.21	D
MOTA	3642	N	ALA	D	82	105.087	29.829	8.079	1.00 34.40	a
ATOM	3643	CA	ALA	D	82	104.294	30.984	7.685	1.00 32.51	D
MOTA	3644	СВ	ALA	D	82	103.915	31.789	8.920	1.00 32.45	D
ATOM	3645	C	ALA		82	105.064	31.866	6.707	1.00 32.78	D
ATOM		ō	ALA		82	106.294	31.913	6.740	1.00 30.87	D
	3646									ם
MOTA	3647	N	THR		83	104.333	32.561	5.839	1.00 32.79	
MOTA	3648	CA	THR		83	104.940	33.459	4.867	1.00 34.48	D
MOTA	3649	CB	THR	D	83	104.195	33.429	3.521	1.00 35.64	α
ATOM	3650	OG1	THR	D	83	104.179	32.094	3.006	1.00 38.88	D
ATOM	3651	CG2	THR	D	83	104.880	34.342	2.521	1.00 35.33	D
ATOM	3652	С	THR	D	83	104.886	34.887	5.401	1.00 35.30	D
MOTA	3653	ō	THR		83	103.827	35.355	5.824	1.00 36.88	D
			ASN		84	106.025	35.575	5.379	1.00 35.07	D
MOTA	3654	N								D
ATOM	3655	CA	asn		84	106.095	36.949	5.855	1.00 33.90	
MOTA	3656	CB	asn		84	107.548	37.413	6.010	1.00 34.23	D
MOTA	3657	CG	asn	D	84	108.351	36.545	6.954	1.00 36.16	D
ATOM	3658	OD1	asn	D	84	107.895	36.195	8.043	1.00 34.99	D
ATOM	3659	ND2	ASN	D	84	109.572	36.205	6.545	1.00 37.40	D
ATOM	3660	C	ASN	D	84	105.419	37.879	4.865	1.00 34.74	D
ATOM	3661	0	ASN		84	105.814	37.940	3.699	1.00 35.59	D
ATOM	3662	N	GLU		85	104.401	38.599	5.327	1.00 34.09	D
								4.489	1.00 32.99	D
MOTA	3663	CA	GLU		85	103.695	39.561			
MOTA	3664	CB	GLU		85	102.239	39.714	4.939	1.00 35.56	D
MOTA	3665	CG	GLU		85	101.370	38.475	4.746	1.00 40.80	D
ATOM	3666	В	GLU	D	85	101.019	38.215	3.291	1.00 43.32	D
MOTA	3667	OE1	GLU	D	85	100.409	39.104	2.658	1.00 46.21	D
MOTA	3668	OB2	GLU	D	85	101.345	37.119	2.782	1.00 44.58	D
ATOM	3669	C	GLU		85	104.418	40.886	4.681	1.00 31.21	D
ATOM	3670	ō	GLU		85	105.220	41.024	5.602	1.00 32.36	D
ATOM	3671	N	VAL		86	104.140	41.848	3.808	1.00 29.71	D
								3.882	1.00 27.94	D
ATOM	3672	CA	VAL		86	104.749	43.170			
ATOM	3673	CB	VAL		86	105.079	43.712	2.467	1.00 26.90	D
ATOM	3674		. VAL		86	105.569	45.166	2.543	1.00 23.11	D
MOTA	3675	CG2	VAL	D	86	106.134	42.829	1.821	1.00 24.31	D
ATOM	3676	С	VAL	D	86	103.767	44.114	4.574	1.00 29.81	D
ATOM	3677	0	VAL	D	86	102.658	44.343	4.088	1.00 30.28	D
MOTA	3678	N	PRO		87	104.162	44.666	5.729	1.00 29.08	D
ATOM	3679	CD	PRO		87	105.356	44.310	6.509	1.00 29.37	D
		CA	PRO		87	103.306	45.583	6.485	1.00 30.85	D
MOTA	3680							7.786	1.00 30.80	D
ATOM	3681	CB	PRO		87	104.083	45.791			
MOTA	3682	CG	PRO		87	104.878	44.551	7.920	1.00 30.83	D
MOTA	3683	C	PRO	ם	87	103.049	46.907	5.772	1.00 31.43	D
MOTA	3684	0	PRO	D	87	103.863	47.357	4.968	1.00 31.78	D
MOTA	3685	N	GLU	D	88	101.907	47.517	6.081	1.00 31.85	D
ATOM	3686	CA	GLU		88	101.516	48.808	5.521	1.00 32.77	D
MOTA	3687	CB	GLU		88	100.195	48.687	4.744	1.00 35.18	Đ
							49.960	3.987	1.00 43.00	D
MOTA	3688	CG	GLU		88	99.814				D
MOTA	3689	CD	GLU		88	98.512	49.839	3.205	1.00 46.30	
ATOM	3690		L GLU		88	97.439	49.745	3.837	1.00 47.40	D
ATOM	3691	OE:	GLT		88	98.564	49.840	1.954	1.00 48.25	D
ATOM	3692	C	GL	D	88	101.338	49.748	6.721	1.00 31.26	D
ATOM	3693	0	GLU	D	88	100.556	49.457	7.630	1.00 31.21	D
ATOM	3694	N	VAI		89	102.060	50.864	6.728	1.00 28.43	D
MOTA	3695	CA	VAI		89	101.988	51.806	7.842	1.00 26.87	D
424 Uli	2000				00	104.700				_

ATOM	3696	СВ	VAL D	89	103.385	52.024	8.454	1.00 26.58	D
ATOM	3697		VAL D	89	103.277	52.886	9.699	1.00 26.80	D
ATOM	3698		VAL D	89	104.021	50.679	8.787	1.00 24.58	D
ATOM	3699	C	VAL D	89	101.389	53.174	7.505	1.00 27.02	D
			VAL D		101.698	53.772	6.473	1.00 26.22	D
ATOM	3700	0		89				1.00 26.33	D
MOTA	3701	N	THR D	90	100.530	53.662	8.394 8.219		D
ATOM	3702	CA	THR D	90	99.881	54.955		1.00 26.05	
ATOM	3703	CB	THR D	90	98.414	54.802	7.769	1.00 27.24	D
MOTA	3704		THR D	90	98.359	54.063	6.543	1.00 31.41	D
MOTA	3705	CG2	THR D	90	97.786	56.163	7.545	1.00 28.57	D
ATOM	3706	C	THR D	90	99.883	55.698	9.546	1.00 24.83	D
MOTA	3707	0	THR D	90	99.542	55.120	10.581	1.00 25.45	D
ATOM	3708	N	VAL D	91	100.266	56.972	9.512	1.00 22.04	D
ATOM	3709	CA	VAL D	91	100.300	57.791	10.716	1.00 21.50	D
ATOM	3710	CB	VAL D	91	101.749	58.280	11.031	1.00 23.04	D
ATOM	3711	CG1	VAL D	91	101.737	59.245	12.225	1.00 22.74	D
ATOM	3712	CG2	VAL D	91	102.650	57.082	11.340	1.00 20.38	ם
ATOM	3713	C	VAL D	91	99.369	58.993	10.553	1.00 21.65	D
ATOM	3714	0	VAL D	91	99.357	59.653	9.509	1.00 21.70	D
ATOM	3715	N	PHE D	92	98.573	59.252	11.586	1.00 21.34	D
ATOM	3716	CA	PHE D	92	97.633	60.363	11.580	1.00 21.48	D
ATOM	3717	СВ	PHE D	92	96.370	59.985	10.788	1.00 21.60	D
			PHE D	92	95.652	58.771	11.314	1.00 22.22	D
ATOM	3718	CG						1.00 24.10	Ď
ATOM	3719		PHE D	92	94.601	58.902	12.215		
MOTA	3720		DHE D	92	96.038	57.495	10.925	1.00 24.53	D
ATOM	3721		PHE D	92	93.940	57.774	12.724	1.00 22.72	D
ATOM	3722	CE2	PHE D	92	95.386	56.355	11.428	1.00 23.87	D
MOTA	3723	CZ	PHE D	92	94.335	56.501	12.329	1.00 21.18	D
MOTA	3724	C	PHE D	92	97.303	60.700	13.030	1.00 22.72	D
ATOM	3725	0	PHE D	92	97.607	59.921	13.933	1.00 22.31	D
MOTA	3726	N	SER D	93	96.696	61.859	13.261	1.00 22.45	D
ATOM	3727	CA	SER D	93	96.366	62.262	14.623	1.00 21.69	D
ATOM	3728	CB	SER D	93	96.599	63.764	14.799	1.00 20.96	D
ATOM	3729	OG	SER D	93	95.696	64.508	14.010	1.00 25.08	D
ATOM	3730	C	SER D	93	94.931	61.913	14.990	1.00 21.02	D
MOTA	3731	ō	SER D	93	94.078	61.755	14.127	1.00 20.62	D
ATOM	3732	N	LYS D	94	94.676	61.791	16.283	1.00 20.66	D
ATOM	3733	CA	LYS D	94	93.350	61.453	16.768	1.00 24.11	D
ATOM	3734	СВ	LYS D	94	93.444	60.985	18.223	1.00 24.91	D
ATOM	3735	CG	LYS D	94	92.121	60.605	18.865	1.00 29.49	Ø
			LYS D	94	92.353	60.101	20.293	1.00 32.97	D
MOTA	3736	CD				59.909	21.052	1.00 33.37	D
ATOM	3737	CE	LYS D	94	91.050		20.399	1.00 34.08	Ď
MOTA	3738	NZ	LYS D	94	90.175	58.897	16.654	1.00 24.40	Ď
ATOM	3739	C	LYS D	94	92.406	62.646		1.00 24.40	Ď
MOTA	3740	0	LYS D	94	91.224	62.495	16.356		D
ATOM	3741	N	SER D	95	92.935	63.834	16.894	1.00 25.54 1.00 29.22	D
MOTA	3742	CA	SER D	95	92.133	65.040	16.815		
ATOM	3743	CB	SER D	95	91.932	65.643	18.208	1.00 30.47	D
MOTA	3744	OG	SER D	95	91.236	64.746	19.060	1.00 36.11	D
ATOM	3745	C	SER D	95	92.843	66.046	15.932	1.00 29.71	D
MOTA	3746	0	SER D	95	93.993	65.834	15.531	1.00 29.68	D
MOTA	3747	N	PRO D	96	92.159	67.146	15.588	1.00 29.93	D
MOTA	3748	CD	PRO D	96	90.760	67.532	15.843	1.00 31.14	D
MOTA	3749	CA	PRO D	96	92.836	68.129	14.747	1.00 29.29	D
MOTA	3750	CB	PRO D	96	91.714	69.097	14.369	1.00 31.65	D
MOTA	3751	CG	PRO D	96	90.777	69.010	15.545	1.00 30.66	D
ATOM	3752	C	PRO D		93.939	68.765	15.587	1.00 27.35	D
ATOM	3753	ō	PRO D		93.818	68.904	16.806	1.00 24.86	D
MOTA	3754	N	VAL D		95.025	69.127	14.929	1.00 26.81	D
MOTA	3755	CA	VAL D		96.158	69.706	15.615	1.00 29.25	D
ATOM	3756	CB	VAL D		97.438	69.501	14.783	1.00 31.49	D
			VAL D		98.652	69.998	15.556	1.00 33.50	D
MOTA	3757							1.00 34.03	D
MOTA	3758		VAL D		97.583	68.029	14.415 15.910	1.00 28.80	D
ATOM	3759	C	VAL D		96.007	71.196		1.00 28.78	
MOTA	3760	0	VAL D		95.749	71.998	15.012		D D
MOTA	3761	N	THR D		96.144	71.559	17.178	1.00 27.47	
ATOM	3762	CA	THR D		96.091	72.960	17.572	1.00 26.55	D
MOTA	3763	CB	THR D		94.723	73.365	18.209	1.00 26.16	D
ATOM	3764		L THR C		94.684	72.961	19,575	1.00 31.83	D
MOTA	3765	CG2			93.567	72.717	17.469	1.00 23.66	D
MOTA	3766	C	THR I		97.220		18.581	1.00 25.73	D
MOTA	3767	0	THR I		97.260	72.412	19.591	1.00 27.12	D
MOTA	3768	N	LEU I	99	98.159	74.005	18.285	1.00 26.12	D
ATOM	3769	CA	LEU I	99	99.307	74.236	19.156	1.00 27.47	D

NOTICE N										
ATOM 3772 CDI LEBU D 99 101.458 76.607 26.501 1.00 35.00 D ATOM 3774 CD LEBU D 99 98.935 74.416 20.021 1.00 26.088 D ATOM 3776 N GLIN D 99 98.935 74.416 20.021 1.00 25.08 D ATOM 3776 N GLIV D 100 99.585 73.684 21.500 1.00 26.03 D ATOM 3778 C GLIV D 100 99.585 73.684 21.924 1.00 26.02 D ATOM 3780 O GLIV D 101 99.585 73.684 21.212 1.00 26.02 D ATOM 3780 O GLIV D 101 95.537 71.297 21.727 1.00 22.24 D ATOM 3786 CAS COLIN D 101 95.57 71.297 21.50 <th< td=""><td>ATOM</td><td>3770</td><td>CB</td><td>LEU D</td><td>99</td><td>100.089</td><td>75.459</td><td>18.675</td><td>1.00 31.04</td><td>D</td></th<>	ATOM	3770	CB	LEU D	99	100.089	75.459	18.675	1.00 31.04	D
ATOM 3772 CDI LEBU D 99 101.458 76.607 26.501 1.00 35.00 D ATOM 3774 CD LEBU D 99 98.935 74.416 20.021 1.00 26.088 D ATOM 3776 N GLIN D 99 98.935 74.416 20.021 1.00 25.08 D ATOM 3776 N GLIV D 100 99.585 73.684 21.500 1.00 26.03 D ATOM 3778 C GLIV D 100 99.585 73.684 21.924 1.00 26.02 D ATOM 3780 O GLIV D 101 99.585 73.684 21.212 1.00 26.02 D ATOM 3780 O GLIV D 101 95.537 71.297 21.727 1.00 22.24 D ATOM 3786 CAS COLIN D 101 95.57 71.297 21.50 <th< td=""><td>ATOM</td><td>3771</td><td>CG</td><td>PEA D</td><td>99</td><td>100.758</td><td>75.309</td><td>17.310</td><td>1.00 33.09</td><td>D</td></th<>	ATOM	3771	CG	PEA D	99	100.758	75.309	17.310	1.00 33.09	D
NOTE										
NATION 3774 C										
NTOM 3775 O LEUD D 99 99.077 75.222 20.946 1.00 25.97 D	ATOM	3773	CD2	PEA D	99	101.754				
ATOM 3776 N GIAY D 99.585 73.654 21.590 1.00 26.93 D ATOM 3778 C GIAY D 100 98.233 72.798 22.422 1.00 26.02 D ATOM 3780 C GIAY D 100 98.203 72.622 24.622 1.00 25.51 D ATOM 3781 C GIAY D 100 95.5372 72.143 22.491 1.00 25.51 D ATOM 3781 CA GIAY D 100 95.372 71.297 21.256 1.00 25.51 D ATOM 3784 CB GIAY D 100 95.372 71.299 22.1776 1.00 23.24 D ATOM 3786 NEZ GIAY D 101 96.9756 97.539 91.551 1.00 24.108 D ATOM 3786 NEZ GIAY D 101 93.515 69.345 21.057	MOTA	3774	C	PEA D	99	98.935	74.416	20.621	1.00 26.08	Ð
ATOM 3776 N GIAY D 99.585 73.654 21.590 1.00 26.93 D ATOM 3778 C GIAY D 100 98.233 72.798 22.422 1.00 26.02 D ATOM 3780 C GIAY D 100 98.203 72.622 24.622 1.00 25.51 D ATOM 3781 C GIAY D 100 95.5372 72.143 22.491 1.00 25.51 D ATOM 3781 CA GIAY D 100 95.372 71.297 21.256 1.00 25.51 D ATOM 3784 CB GIAY D 100 95.372 71.299 22.1776 1.00 23.24 D ATOM 3786 NEZ GIAY D 101 96.9756 97.539 91.551 1.00 24.108 D ATOM 3786 NEZ GIAY D 101 93.515 69.345 21.057	ATOM	3775	0	TEO D	99	98.077	75.222	20.946	1.00 25.97	D
ATOM 3777 CA GIAY D 100 99.310 73.749 22.924 1.00 26.03 D 100 M 1778 C GIAY D 100 98.020 72.662 24.629 1.00 25.51 D 100 98.020 72.662 24.629 1.00 25.51 D 100 98.020 72.662 24.629 1.00 25.51 D 100 96.480 71.199 22.820 1.00 26.03 D 100 100 97.551 72.132 22.491 1.00 25.51 D 100 100 97.551 72.132 22.491 1.00 25.51 D 100 100 97.551 72.132 22.491 1.00 25.51 D 100 100 94.600 69.459 20.115 1.00 31.65 D 100 100 95.760 69.388 19.511 1.00 31.68 D 100 100 95.760 69.388 19.511 1.00 31.81 D 100 100 95.760 69.585 69.508 22.861 1.00 22.22 D 100 100 100 95.649 69.545 22.861 1.00 22.22 D 100 100 100 95.649 69.545 22.861 1.00 22.22 D 100 100 100 95.649 66.845 23.015 1.00 22.76 D 100 100 95.650 69.33 65.25 23.09 1.00 10.630 D 100 95.650 66.845 23.015 1.00 22.76 D 100 100 95.650 66.845 23.015 1.00 22.76 D 100 100 95.650 66.845 23.015 1.00 22.76 D 100 100 95.84 D 100 100 95.850 66.950 100 100 95.850 66.950 100 100 95.850										
NET										
NATION 1779 O GILY D 100 98.020 72.662 24.629 1.00 25.51 D NATION 3780 N GLN D 101 97.553 72.142 22.491 1.00 25.73 D NATION 3782 C8 GLN D 101 96.490 71.199 22.820 1.00 28.13 D NATION 3782 C8 GLN D 101 94.6617 69.991 21.560 1.00 36.65 D NATION 3785 OEI GLN D 101 94.6617 69.991 21.560 1.00 36.65 D NATION 3785 OEI GLN D 101 94.6617 69.491 20.115 1.00 41.00 D NATION 3786 OEI GLN D 101 95.760 69.388 19.511 1.00 38.18 D NATION 3787 C GLN D 101 95.760 69.388 19.511 1.00 38.18 D NATION 3787 C GLN D 101 97.477 69.245 22.615 1.00 25.22 D NATION 3788 N PRD D 102 96.485 69.544 25.343 1.00 24.55 D NATION 3798 O GLN D 102 96.485 69.544 25.343 1.00 24.25 D NATION 3799 CA PRD D 102 96.486 69.544 25.343 1.00 22.22 D NATION 3791 CA PRD D 102 96.649 66.845 23.616 1.00 22.02 D NATION 3793 CA PRD D 102 96.649 66.845 23.616 1.00 22.02 D NATION 3795 O PRD D 102 96.649 66.845 23.615 1.00 22.02 D NATION 3797 CA ASN D 103 97.409 66.055 22.264 1.00 22.05 D NATION 3797 CA ASN D 103 97.409 66.055 22.264 1.00 22.65 D NATION 3797 CA ASN D 103 97.409 66.055 22.264 1.00 12.65 D NATION 3797 CA ASN D 103 97.559 64.946 66.845 23.614 1.00 10.630 D NATION 3797 CA ASN D 103 97.409 66.055 22.264 1.00 12.65 D NATION 3797 CA ASN D 103 97.409 66.055 22.264 1.00 12.65 D NATION 3804 N LIE D 104 97.405 63.805 21.248 1.00 16.30 D NATION 3808 CA LIE D 104 97.405 63.805 21.248 1.00 16.30 D NATION 3808 CA LIE D 104 97.405 63.805 21.248 1.00 17.24 D NATION 3808 CA LIE D 104 96.807 60.277 12.595 1.00 17.15 D NATION 3	ATOM	3777	CA	GLY D	100	99.310	73.749			
NATION 3780 N GIN D 101 97.553 72.143 22.491 1.00 25.73 D NATION 3781 CA GIN D 101 95.372 71.297 21.776 1.00 22.24 D NATION 3783 CS GIN D 101 94.680 69.981 21.560 1.00 28.18 D NATION 3785 CS GIN D 101 95.372 71.297 21.776 1.00 22.24 D NATION 3785 GIN D 101 95.760 69.981 21.560 1.00 28.18 D NATION 3786 RIZ GIN D 101 95.760 69.381 91.551 1.00 41.08 D NATION 3787 GIN D 101 95.760 69.381 91.551 1.00 41.08 D NATION 3788 O GIN D 101 97.477 69.282 22.861 1.00 25.22 D NATION 3789 O GIN D 101 97.477 69.282 22.861 1.00 25.22 D NATION 3790 CD PRO D 102 96.885 69.078 24.089 1.00 22.76 D NATION 3791 CA PRO D 102 97.359 67.683 24.080 1.00 22.76 D NATION 3792 CB PRO D 102 97.688 68.542 26.343 1.00 22.22 D NATION 3795 O PRO D 102 97.688 68.542 26.343 1.00 22.72 D NATION 3795 O PRO D 102 97.688 68.542 26.343 1.00 22.02 D NATION 3795 O PRO D 102 97.688 68.542 22.874 1.00 22.02 D NATION 3795 O PRO D 102 97.688 68.542 22.876 1.00 22.44 D NATION 3795 O PRO D 102 95.649 66.495 23.915 1.00 21.72 D NATION 3795 O PRO D 102 95.649 66.495 23.915 1.00 21.72 D NATION 3795 O PRO D 102 95.649 66.495 23.915 1.00 21.76 D NATION 3795 O PRO D 102 95.649 66.495 23.915 1.00 21.76 D NATION 3795 O PRO D 102 95.649 66.495 23.915 1.00 21.78 D NATION 3801 O D NATION 3801 O D NATION 3801 O D NATION 3801 O D NATION 3805 O RATION 3801 O D RATION 3802 O RATION 3805 CA LIE D 104 96.402 C 66.823 1.00 17.69 D D RATION 3805 CA LIE D	ATOM	3778	C	GLY D	100	98.233	72.798	23.422	1.00 26.02	D
NATION 3780 N GIN D 101 97.553 72.143 22.491 1.00 25.73 D NATION 3781 CA GIN D 101 95.372 71.297 21.776 1.00 22.24 D NATION 3783 CS GIN D 101 94.680 69.981 21.560 1.00 28.18 D NATION 3785 CS GIN D 101 95.372 71.297 21.776 1.00 22.24 D NATION 3785 GIN D 101 95.760 69.981 21.560 1.00 28.18 D NATION 3786 RIZ GIN D 101 95.760 69.381 91.551 1.00 41.08 D NATION 3787 GIN D 101 95.760 69.381 91.551 1.00 41.08 D NATION 3788 O GIN D 101 97.477 69.282 22.861 1.00 25.22 D NATION 3789 O GIN D 101 97.477 69.282 22.861 1.00 25.22 D NATION 3790 CD PRO D 102 96.885 69.078 24.089 1.00 22.76 D NATION 3791 CA PRO D 102 97.359 67.683 24.080 1.00 22.76 D NATION 3792 CB PRO D 102 97.688 68.542 26.343 1.00 22.22 D NATION 3795 O PRO D 102 97.688 68.542 26.343 1.00 22.72 D NATION 3795 O PRO D 102 97.688 68.542 26.343 1.00 22.02 D NATION 3795 O PRO D 102 97.688 68.542 22.874 1.00 22.02 D NATION 3795 O PRO D 102 97.688 68.542 22.876 1.00 22.44 D NATION 3795 O PRO D 102 95.649 66.495 23.915 1.00 21.72 D NATION 3795 O PRO D 102 95.649 66.495 23.915 1.00 21.72 D NATION 3795 O PRO D 102 95.649 66.495 23.915 1.00 21.76 D NATION 3795 O PRO D 102 95.649 66.495 23.915 1.00 21.76 D NATION 3795 O PRO D 102 95.649 66.495 23.915 1.00 21.78 D NATION 3801 O D NATION 3801 O D NATION 3801 O D NATION 3801 O D NATION 3805 O RATION 3801 O D RATION 3802 O RATION 3805 CA LIE D 104 96.402 C 66.823 1.00 17.69 D D RATION 3805 CA LIE D	ATOM	3779	0	GLY D	100	98.020	72.662	24.629	1.00 25.51	D
Name										
NOTE 1982 CR CIN D 101 95.372 71.297 21.776 1.00 32.24 D										
NOTICE 1988 1988 1988 1988 1988 1988 1988 1888	ATOM	3781	CA	GLN D	101	96.490	71.199	22.820	1.00 28.13	
NTOM 3784 CD CLN D LOL 94	ATOM	3782	CB	GLN D	101	95.372	71.297	21.776	1.00 32.24	D
NTOM 3784 CD CLN D LOL 94	ATOM	3783	CG	GLN D	101	94.617	69.981	21.560	1.00 38.65	D
ATOM 3785										
ATOM 3786 NEZ CLN D D D S S S S S S S										
ATOM 3787 C GLAN D 101 96.994 69.756 22.861 1.00 25.22 D ATOM 3788 O GLN D 101 97.477 69.245 21.857 1.00 24.55 D ATOM 3789 N PRO D 102 96.885 69.578 24.019 1.00 24.18 D ATOM 3790 CD PRO D 102 96.885 69.578 24.039 1.00 22.75 D ATOM 3791 CA PRO D 102 96.885 69.578 24.080 1.00 22.75 D ATOM 3791 CA PRO D 102 96.885 69.544 25.343 1.00 22.72 D ATOM 3792 CB PRO D 102 96.939 67.253 25.494 1.00 22.02 D ATOM 3793 CG PRO D 102 96.693 67.253 25.494 1.00 22.02 D ATOM 3793 CG PRO D 102 96.693 67.253 25.494 1.00 22.02 D ATOM 3794 C PRO D 102 96.649 66.845 23.015 1.00 21.72 D ATOM 3795 O PRO D 102 96.649 66.845 23.015 1.00 21.72 D ATOM 3795 O PRO D 102 96.649 66.925 22.2676 1.00 21.72 D ATOM 3795 O PRO D 103 97.409 66.055 22.2676 1.00 21.78 D ATOM 3795 CB ASN D 103 97.412 65.556 19.838 1.00 16.30 D ATOM 3798 CB ASN D 103 97.412 65.556 19.838 1.00 16.30 D ATOM 3798 CB ASN D 103 97.112 65.556 19.838 1.00 16.30 D ATOM 3798 CB ASN D 103 96.035 65.857 18.824 1.00 16.50 D ATOM 3799 CG ASN D 103 96.555 66.643 18.160 1.00 14.61 D ATOM 3800 ODI ASN D 103 95.552 66.643 18.160 1.00 14.61 D ATOM 3800 CD ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3804 N ILE D 104 97.010 62.977 20.284 1.00 17.24 D ATOM 3806 CB ILE D 104 97.010 62.977 20.284 1.00 17.39 D ATOM 3806 CB ILE D 104 97.465 61.595 20.198 1.00 17.39 D ATOM 3807 CG ILE D 104 96.826 51.557 20.498 1.00 17.39 D ATOM 3807 CG ILE D 104 96.826 51.557 20.498 1.00 17.39 D ATOM 3807 CG ILE D 104 96.881 53.175 20.498 1.00 17.39 D ATOM 3807 CG ILE D 104 96.881 53.175 20.498 1.00 17.98 D ATOM 3807 CG ILE D 104 96.881 53.175 20.498 1.00 17.98 D ATOM 3807 CG ILE D 104 96.881 53.175 20.498 1.00 17.98 D ATOM 3810 C ILE D 104 96.881 53.175 20.498 1.00 17.98 D ATOM 3810 C ILE D 104 96.881 53.175 20.498 1.00 17.98 D ATOM 3811 C ILE D 104 96.881 53.175 20.498 1.00 17.98 D ATOM 3812 C ILE D 104 96.887 53.985 1.00 18.07 D ATOM 3813 C ILE D 105 90.985 1.00 18.07 D 17.99 1.00 18.07 D ATOM 3813 C ILE D 106 96.895 57.595 1.00 10.10 10.10 10.10 10.10 10.10 10.10 10.10 10.10 10.10 10.10 10.10 10.10 10.10	ATOM	3785	OEI	GLN D	101		69.348			
ATOM 3787 C GIN D 101 96.994 69.756 22.861 1.00 25.22 D ATOM 3790 N FRO D 102 96.885 69.078 24.019 1.00 24.55 D ATOM 3790 CD FRO D 102 96.885 69.078 24.019 1.00 24.55 D ATOM 3791 CA FRO D 102 97.359 67.683 24.080 1.00 22.22 D ATOM 3791 CA FRO D 102 96.963 67.253 25.494 1.00 22.02 D ATOM 3793 CG FRO D 102 96.963 67.253 25.494 1.00 22.02 D ATOM 3793 CG FRO D 102 96.696 66.845 23.015 1.00 21.72 D ATOM 3795 CD FRO D 102 96.696 66.845 23.015 1.00 21.72 D ATOM 3795 CD FRO D 102 96.496 66.845 23.015 1.00 21.72 D ATOM 3795 CD FRO D 102 96.699 66.925 22.2676 1.00 21.72 D ATOM 3795 CD FRO D 102 96.699 66.925 22.2676 1.00 19.84 D ATOM 3797 CA ASIN D 103 97.409 66.055 22.2676 1.00 17.89 D ATOM 3797 CA ASIN D 103 97.410 65.925 12.09 1.00 17.89 D ATOM 3798 CB ASIN D 103 97.410 65.825 12.09 1.00 17.89 D ATOM 3799 CG ASIN D 103 97.410 65.825 12.09 1.00 17.89 D ATOM 3799 CG ASIN D 103 95.552 64.446 18.636 1.00 16.50 D ATOM 3800 ODI ASIN D 103 95.552 64.446 18.636 1.00 16.50 D ATOM 3800 ODI ASIN D 103 95.552 64.446 18.636 1.00 16.50 D ATOM 3800 C ASIN D 103 95.552 64.446 18.636 1.00 14.61 D ATOM 3800 ODI ASIN D 103 95.552 64.446 18.636 1.00 14.61 D ATOM 3800 ODI ASIN D 103 95.552 64.446 18.636 1.00 16.80 D ATOM 3800 ODI ASIN D 103 95.552 64.446 18.636 1.00 14.61 D ATOM 3806 CB ILE D 104 97.010 62.977 20.284 1.00 17.24 D ATOM 3806 CB ILE D 104 97.010 62.977 20.284 1.00 17.24 D ATOM 3806 CB ILE D 104 96.402 60.627 20.755 1.00 17.39 D ATOM 3806 CB ILE D 104 96.402 60.627 20.755 1.00 17.98 D ATOM 3806 CB ILE D 104 96.402 60.627 20.755 1.00 17.99 D ATOM 3806 CB ILE D 104 96.402 60.627 20.755 1.00 17.95 D ATOM 3815 CG ILE D 104 96.807 60.627 17.77 1.00 17.95 D ATOM 3815 CG ILE D 104 96.807 60.627 17.77 1.00 17.95 D ATOM 3815 CG ILE D 104 96.807 60.627 17.77 1.00 18.46 D ATOM 3815 CG ILE D 104 96.807 60.627 17.77 1.00 18.07 D ATOM 3816 CD ILE D 105 90.807 60.727 17.77 1.00 18.07 D ATOM 3816 CD ILE D 106 90.807 50.807 18.807 10.00 17.14 D ATOM 3816 CD ILE D 106 90.807 50.807 18.807 10.00 17.14 D ATOM 3816 CD ILE D 106 90.807 50.807 18.8	ATOM	3786	NE2	GLN D	101	93.515	69.119	19.566	1.00 40.87	D
ATOM 3789 N		3787	C	GLN D	101	96.994	69.756	22.861	1.00 25.22	D
ATOM 3789 N FRO D 102 96.885 69.078 24.019 1.00 24.18 D ATOM 3790 CD FRO D 102 96.436 69.544 25.343 1.00 22.22 D ATOM 3791 CA PRO D 102 96.936 67.553 25.494 1.00 22.02 D ATOM 3792 CB FRO D 102 96.936 67.253 25.494 1.00 22.02 D ATOM 3793 CG PRO D 102 96.693 67.253 25.494 1.00 22.02 D ATOM 3794 C PRO D 102 96.649 66.845 23.015 1.00 21.72 D ATOM 3795 O PRO D 102 96.649 66.845 23.015 1.00 21.72 D ATOM 3795 O PRO D 102 96.649 66.845 23.015 1.00 21.72 D ATOM 3795 O PRO D 102 96.649 66.845 23.015 1.00 21.72 D ATOM 3795 O PRO D 102 96.649 66.845 23.015 1.00 21.72 D ATOM 3797 CA ASN D 103 97.409 66.055 22.2676 1.00 19.84 D ATOM 3797 CG ASN D 103 97.409 66.055 22.266 1.00 19.84 D ATOM 3797 CG ASN D 103 96.803 65.255 21.209 1.00 17.89 D ATOM 3798 CB ASN D 103 97.112 65.856 19.838 1.00 16.30 D ATOM 3798 CG ASN D 103 96.555 66.643 18.636 1.00 16.80 D ATOM 3800 ODI ASN D 103 95.552 66.446 18.636 1.00 16.80 D ATOM 3801 NDZ ASN D 103 95.559 66.643 18.636 1.00 17.24 D ATOM 3801 NDZ ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3803 O ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3803 O ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3805 CB ILE D 104 97.055 66.543 18.160 1.00 17.24 D ATOM 3805 CB ILE D 104 97.055 61.555 10.98 1.00 17.24 D ATOM 3805 CB ILE D 104 97.455 61.555 20.98 1.00 17.39 D ATOM 3805 CB ILE D 104 96.818 59.175 20.498 1.00 17.39 D ATOM 3805 CB ILE D 104 96.818 59.175 20.498 1.00 17.39 D ATOM 3805 CB ILE D 104 96.818 59.175 20.498 1.00 17.98 D ATOM 3810 C ILE D 104 97.765 61.555 20.98 1.00 17.98 D ATOM 3810 C ILE D 104 97.765 61.555 20.98 1.00 17.98 D ATOM 3810 C ILE D 104 97.765 61.555 20.98 1.00 17.98 D ATOM 3811 O ILE D 104 97.765 61.555 20.98 1.00 17.98 D ATOM 3810 C ILE D 104 97.765 61.555 20.98 1.00 17.98 D ATOM 3810 C ILE D 104 97.765 61.555 20.98 1.00 17.98 D ATOM 3810 C ILE D 104 97.765 61.555 20.98 1.00 17.98 D ATOM 3810 C ILE D 104 97.765 61.555 20.98 1.00 17.98 D ATOM 3810 C ILE D 105 99.366 61.555 20.99 1.00 18.75 D ATOM 3810 C ILE D 105 99.366 61.555 20.99 1.00 18.75 D ATOM 3810 C ILE D 10										
ATOM 3790 CD PRO D 102 96.436 69.544 25.343 1.00 22.276 D ATOM 3791 CD PRO D 102 97.359 67.683 24.080 1.00 22.76 D D ATOM 3793 CG PRO D 102 97.088 68.542 26.274 1.00 22.02 D ATOM 3793 CG PRO D 102 97.088 68.542 26.274 1.00 22.07 D ATOM 3793 C PRO D 102 95.693 67.283 25.494 1.00 22.07 D ATOM 3795 C PRO D 102 95.649 66.845 23.015 1.00 21.72 D ATOM 3795 N ASN D 103 95.649 66.845 23.015 1.00 21.72 D ATOM 3795 N ASN D 103 97.409 66.955 22.264 1.00 19.84 D ATOM 3795 N ASN D 103 96.833 65.225 21.209 1.00 17.89 D ATOM 3797 CA ASN D 103 96.833 65.225 21.209 1.00 17.89 D ATOM 3799 CG ASN D 103 96.005 65.856 19.838 1.00 16.30 D ATOM 3799 CG ASN D 103 95.552 64.446 18.636 1.00 16.80 D ATOM 3800 ODI ASN D 103 95.552 64.446 18.636 1.00 16.80 D ATOM 3800 ODI ASN D 103 95.552 64.446 18.636 1.00 14.61 D ATOM 3800 CG ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3803 C ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3805 CA ILE D 104 97.010 62.977 20.284 1.00 15.74 D ATOM 3805 CA ILE D 104 97.405 61.595 20.198 1.00 15.74 D ATOM 3805 CA ILE D 104 97.405 61.595 20.198 1.00 15.30 D ATOM 3806 CB ILE D 104 96.402 60.627 20.755 1.00 17.89 D ATOM 3806 CD ILE D 104 96.202 60.866 22.253 1.00 18.46 D ATOM 3805 CD ILE D 104 96.202 60.867 20.255 1.00 17.89 D ATOM 3805 CD ILE D 104 96.202 60.867 20.255 1.00 17.89 D ATOM 3810 C ILE D 104 97.760 61.855 18.873 1.00 17.15 D ATOM 3811 O ILE D 104 96.202 60.867 20.255 1.00 17.89 D ATOM 3812 N ILE D 104 96.202 60.867 20.255 1.00 17.15 D ATOM 3812 N ILE D 104 96.202 60.867 20.255 1.00 17.15 D ATOM 3811 O ILE D 104 96.807 61.855 18.864 1.00 17.15 D ATOM 3811 O ILE D 104 96.807 61.855 18.864 1.00 17.15 D ATOM 3812 N ILE D 104 96.807 61.855 18.864 1.00 17.15 D ATOM 3812 N ILE D 105 99.370 60.272 17.177 1.00 16.66 D ATOM 3813 CA ILE D 105 99.366 60.272 17.177 1.00 16.65 D ATOM 3815 CD ILE D 105 99.366 50.255 12.50 17.14 D ATOM 3815 CD ILE D 106 96.807 61.385 18.903 1.00 17.14 D ATOM 3820 N ILE D 106 96.807 61.385 18.903 1.00 17.14 D ATOM 3820 CD ILE D 106 96.807 55.325 18.800 17.14 D ATOM 3820 C ILE										
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ATOM 3792 CB PRO D 102 96.983 67.253 25.494 1.00 22.02 D ATOM 3793 CG PRO D 102 97.088 68.542 26.274 1.00 22.44 D ATOM 3794 C PRO D 102 95.649 66.845 23.015 1.00 21.72 D ATOM 3795 O PRO D 102 95.429 66.922 22.867 1.00 22.65 D ATOM 3795 N ASN D 103 97.409 66.055 22.264 1.00 19.84 D ATOM 3795 N ASN D 103 97.409 66.055 22.264 1.00 19.84 D ATOM 3797 CA ASN D 103 97.409 66.055 22.264 1.00 19.84 D ATOM 3797 CA ASN D 103 97.112 65.856 19.838 1.00 16.30 D ATOM 3799 CG ASN D 103 95.552 64.446 18.636 1.00 16.80 D ATOM 3800 OD1 ASN D 103 95.552 64.446 18.636 1.00 16.80 D ATOM 3801 ND2 ASN D 103 95.552 66.643 18.100 17.24 D ATOM 3802 C ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3803 O ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3805 CA LIE D 104 97.405 66.057 20.284 1.00 17.39 D ATOM 3805 CA LIE D 104 97.405 66.057 20.284 1.00 17.39 D ATOM 3806 CB LIE D 104 97.465 61.555 20.198 1.00 17.39 D ATOM 3806 CB LIE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3808 CG1 LIE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3808 CG1 LIE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3801 CL LIE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3801 C LIE D 104 96.818 59.175 20.498 1.00 17.59 D ATOM 3801 C LIE D 104 96.818 59.175 20.498 1.00 17.59 D ATOM 3801 C LIE D 104 96.818 59.175 20.498 1.00 17.59 D ATOM 3801 C LIE D 104 96.818 59.175 20.498 1.00 17.59 D ATOM 3810 C LIE D 104 96.818 59.175 20.498 1.00 17.59 D ATOM 3811 C LIE D 104 96.886 61.283 17.902 1.00 18.07 D ATOM 3810 C LIE D 104 96.886 61.283 17.902 1.00 18.07 D ATOM 3810 C LIE D 104 96.886 61.283 17.902 1.00 18.07 D ATOM 3811 C LIE D 105 99.967 61.272 11.55 1.00 18.66 D ATOM 3812 C LIE D 105 99.967 61.287 11.55 1.00 17.55 D ATOM 3816 C LIE D 105 99.967 61.287 11.50 1.00 17.55 D ATOM 3816 C LIE D 105 99.968 58.056 18.056 10.00 17.15 D ATOM 3817 CD2 LIE D 105 99.968 58.056 18.056 10.00 17.14 D ATOM 3820 C LIE D 106 98.875 57.016 15.889 10.00 17.14 D ATOM 3820 C LIE D 106 98.875 57.016 15.889 10.00 17.14 D ATOM 3821 C LIE D 106 98.687 57.016 15.889 10.00 17.14 D ATOM 3821 C L	ATOM	3790	CD	PRO D	102	96.436	69.544	25.343	1.00 22.22	D
ATOM 3792 CB PRO D 102 96.983 67.253 25.494 1.00 22.02 D	MOTA	3791	CA	PRO D	102	97.359	67.683	24.080	1.00 22.76	D
ATOM 3793 CG PRO D 102 97.088 68.542 26.274 1.00 22.444 D ATOM 3795 C PRO D 102 95.429 66.945 23.015 1.00 21.72 D ATOM 3795 O PRO D 102 95.429 66.922 22.876 1.00 22.65 D ATOM 3795 N ASN D 103 97.409 66.055 22.264 1.00 19.84 D ATOM 3797 CA ASN D 103 97.409 66.055 22.264 1.00 19.84 D ATOM 3797 CA ASN D 103 97.409 66.055 22.264 1.00 19.84 D ATOM 3798 CB ASN D 103 97.112 65.856 19.838 1.00 16.30 D ATOM 3798 CB ASN D 103 97.112 65.856 19.838 1.00 16.30 D ATOM 3800 ODI ASN D 103 95.559 66.644 18.636 1.00 16.80 D ATOM 3800 NDI ASN D 103 95.559 66.643 18.160 1.00 14.61 D ATOM 3801 NDI ASN D 103 95.559 66.643 18.160 1.00 14.61 D ATOM 3803 O ASN D 103 97.410 63.805 21.248 1.00 17.39 D ATOM 3803 O ASN D 103 97.410 63.805 21.248 1.00 17.39 D ATOM 3803 O ASN D 103 97.456 61.595 20.198 1.00 15.74 D ATOM 3806 CB ILE D 104 97.465 61.595 20.198 1.00 15.74 D ATOM 3806 CB ILE D 104 96.402 60.627 20.755 1.00 17.89 D ATOM 3808 CG ILE D 104 96.402 60.627 20.755 1.00 17.89 D ATOM 3808 CG ILE D 104 96.402 60.627 20.755 1.00 17.89 D ATOM 3808 CG ILE D 104 96.202 60.866 22.253 1.00 18.46 D ATOM 3801 C ILE D 104 96.185 59.175 20.498 1.00 13.27 D ATOM 3808 CG ILE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3801 C ILE D 104 96.876 61.255 18.763 1.00 17.15 D ATOM 3812 N LEU D 105 98.987 61.223 17.902 1.00 16.66 D ATOM 3812 N LEU D 105 98.987 61.223 17.902 1.00 16.66 D ATOM 3813 CA LEU D 105 99.376 60.272 17.177 1.00 16.65 D ATOM 3813 CA LEU D 105 99.376 60.272 17.177 1.00 16.65 D ATOM 3815 C LEU D 105 99.366 58.085 18.085 1.00 17.86 D ATOM 3815 C LEU D 105 99.366 58.085 18.085 1.00 17.86 D ATOM 3816 CD LEU D 105 99.366 58.085 18.085 1.00 17.86 D ATOM 3819 O LEU D 105 99.366 58.085 18.085 1.00 17.86 D ATOM 3820 N ILE D 106 98.432 58.399 16.099 1.00 16.66 D ATOM 3821 CA LEU D 105 99.366 58.085 18.085 1.00 17.86 D ATOM 3820 N ILE D 106 98.432 58.399 16.099 1.00 17.86 D ATOM 3821 CA LEU D 106 98.432 58.399 15.492 1.00 12.56 D ATOM 3821 CA LEU D 106 98.435 57.015 15.391 1.00 17.86 D ATOM 3821 CA LEU D 106 98.435 57.015 15.391 1.00 19.04 D ATOM										מ
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ATOM 3796 N	ATOM	3795	0	PRO D	102	95.429	66.922	22.876	1.00 22.65	D
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ATOM 3801 ND2 ASN D 103 95.569 66.643 18.160 1.00 14.61 D ATOM 3802 C ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3803 O ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3804 N ILE D 104 97.010 62.977 20.284 1.00 17.39 D ATOM 3805 CA ILE D 104 97.465 61.595 20.198 1.00 17.89 D ATOM 3806 CB ILE D 104 96.806 60.627 20.755 1.00 17.89 D ATOM 3806 CB ILE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3808 CGI ILE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3808 CGI ILE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3809 CDI ILE D 104 95.179 59.965 22.2895 1.00 17.98 D ATOM 3810 C ILE D 104 95.887 60.727 18.509 1.00 17.98 D ATOM 3811 O ILE D 104 97.760 61.185 18.763 1.00 17.15 D ATOM 3812 N LEU D 105 98.987 60.727 18.509 1.00 16.66 D ATOM 3813 CA LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3814 CB LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3816 CDI LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3817 CDZ LEU D 105 102.811 61.994 16.302 1.00 21.66 D ATOM 3818 C LEU D 105 102.811 61.994 16.302 1.00 21.66 D ATOM 3819 O LEU D 105 102.811 61.994 16.302 1.00 21.56 D ATOM 3810 C LEU D 105 99.961 58.804 17.128 1.00 17.13 D ATOM 3812 CA LEU D 105 99.961 58.804 17.128 1.00 17.13 D ATOM 3813 CA LEU D 105 99.961 58.804 17.128 1.00 17.15 D ATOM 3817 CDZ LEU D 105 102.811 61.994 16.302 1.00 21.56 D ATOM 3817 CDZ LEU D 105 99.661 58.804 17.128 1.00 17.18 D ATOM 3817 CDZ LEU D 105 99.661 58.804 17.128 1.00 17.18 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.18 D ATOM 3821 CA ILE D 106 98.432 58.399 16.039 1.00 17.18 D ATOM 3822 CB ILE D 106 98.432 58.399 16.039 1.00 17.18 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.48 D ATOM 3822 CB ILE D 106 98.432 58.399 16.00 17.88 D ATOM 3822 CB ILE D 106 98.431 57.04 11.64 10.0 19.04 D ATOM 3825 CD ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3826 C CILE D 106 98.941 57.004 13.618 1.00 16.48 D ATOM 3826 C CILE D 106 98.941 57.004 13.618 1.00 16.48 D ATOM 3826 C CILE D 108 99.061 58.331 14.700 10.0 19.94 D ATOM 3833 CC CYS D 107 99.634 53.321 14.600 19.94 10.	MOTA	3799	CG	ASN I	103	96.005	65.587	18.824	1.00 16.50	D
ATOM 3801 ND2 ASN D 103 95.569 66.643 18.160 1.00 14.61 D ATOM 3802 C ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3803 O ASN D 103 98.199 63.473 22.129 1.00 15.74 D ATOM 3804 N ILE D 104 97.010 62.977 20.284 1.00 17.39 D ATOM 3805 CA ILE D 104 97.010 62.977 20.284 1.00 17.39 D ATOM 3806 CB ILE D 104 96.402 60.627 20.755 1.00 17.89 D ATOM 3807 CG2 ILE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3809 CD1 ILE D 104 96.820 60.886 22.253 1.00 18.46 D ATOM 3809 CD1 ILE D 104 95.179 59.965 22.895 1.00 17.89 D ATOM 3809 CD1 ILE D 104 97.760 61.185 18.763 1.00 17.15 D ATOM 3811 O ILE D 104 97.760 61.185 18.763 1.00 17.15 D ATOM 3811 O ILE D 104 97.760 61.185 18.763 1.00 17.15 D ATOM 3811 O ILE D 104 95.887 60.272 18.509 1.00 18.07 D ATOM 3813 CA LEU D 105 98.987 60.727 18.509 1.00 16.66 D ATOM 3814 CB LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3815 CG LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3817 CD2 LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3818 CD1 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3818 C LEU D 105 99.370 60.272 15.951 1.00 21.56 D ATOM 3818 C LEU D 105 99.961 58.804 17.128 1.00 17.13 D ATOM 3817 CD2 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3818 C LEU D 105 99.961 58.804 17.128 1.00 17.13 D ATOM 3818 C LEU D 105 99.368 58.056 18.056 1.00 17.13 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.18 D ATOM 3821 CA ILE D 106 98.432 58.399 16.039 1.00 17.18 D ATOM 3822 CB ILE D 106 96.525 56.391 15.492 1.00 17.18 D ATOM 3822 CB ILE D 106 98.432 58.399 16.039 1.00 17.18 D ATOM 3822 CB ILE D 106 98.432 58.399 16.039 1.00 17.19 D ATOM 3824 CG1 ILE D 106 98.876 55.431 14.700 1.00 19.04 D ATOM 3822 CB ILE D 106 98.876 55.431 14.700 1.00 19.04 D ATOM 3823 CG2 ILE D 106 98.876 55.431 14.700 1.00 17.19 D ATOM 3826 C ILE D 106 98.876 55.431 14.700 1.00 17.19 D ATOM 3826 C ILE D 106 98.876 55.312 14.500 1.00 19.04 D ATOM 3826 N CYS D 107 99.634 55.312 14.500 1.00 19.04 D ATOM 3830 CD CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3830 CD CYS D 107 99.632 52.421 14.507 1.00 2	ATOM	3800	OD1	ASN I	103	95.552	64.446	18.636	1.00 16.80	D
ATOM 3802 C ASN D 103 97.410 63.805 21.248 1.00 17.24 D ATOM 3803 O ASN D 103 98.199 63.473 22.129 1.00 15.74 D ATOM 3804 N ILE D 104 97.465 61.595 20.198 1.00 15.30 D ATOM 3805 CA ILE D 104 97.465 61.595 20.198 1.00 15.30 D ATOM 3806 CB ILE D 104 96.402 60.627 20.755 1.00 17.89 D ATOM 3807 CG2 ILE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3808 CG1 ILE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3809 CD1 ILE D 104 96.818 59.175 20.498 1.00 17.98 D ATOM 3809 CD1 ILE D 104 96.887 61.283 17.902 1.00 18.46 D ATOM 3810 C ILE D 104 97.760 61.865 18.763 1.00 17.15 D ATOM 3811 O ILE D 104 96.887 61.283 17.902 1.00 18.07 D ATOM 3812 N LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3813 CA LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3814 CB LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3815 CG LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3816 CD1 LEU D 105 102.811 61.943 16.302 1.00 21.26 D ATOM 3818 C LEU D 105 99.366 58.056 18.056 1.00 21.26 D ATOM 3819 O LEU D 105 99.366 58.056 18.056 1.00 21.26 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3821 CA ILE D 106 96.525 56.939 15.492 1.00 17.14 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 17.44 D ATOM 3823 CG2 ILE D 106 96.525 56.939 15.492 1.00 17.49 D ATOM 3826 C ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3827 CD1 ILE D 106 98.428 57.916 15.839 1.00 17.14 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 C C CYS D 107 99.540 55.312 14.966 1.00 19.74 D ATOM 3829 CA CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3830 C CYS D 107 99.635 53.21 12.493 1.00 19.48 D ATOM 3831 C C LEU D 108 99.077 51.358 10.925 1.00 20.40 D ATOM 3832 CB CYS D 107 99.635 53.21 12.493 1.00 19.48 D ATOM 3833 CC LEU D 108 99.077 51.358 10.925 1.00 20.40 D ATOM 3834 N LEU D 108 99.077 51.358 10.925 1.00 20.40 D ATOM 3836 CD LEU D 108 99.077 51.358 10.925 1.00 20.40 D ATOM 3837 CG LEU D 108 99.077 51.358 10.925 1.00 20.40 D ATOM 3838 CD LEU D 108 99.077 51.145 11.237 1.00 19.64 D ATOM 3834 C LEU D 108 99.077 51.145 11.237 1.00 19.64						95.569	66.643	18.160	1.00 14.61	D
ATOM 3803 O ASN D 103 98.199 63.473 22.129 1.00 15.74 D ATOM 3804 N ILE D 104 97.010 62.977 20.284 1.00 17.39 D ATOM 3805 CA ILE D 104 97.465 61.595 20.198 1.00 15.30 D ATOM 3806 CB ILE D 104 96.402 60.627 20.755 1.00 17.89 D ATOM 3807 CG2 ILE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3808 CG1 ILE D 104 96.202 60.886 22.253 1.00 18.46 D ATOM 3809 CD1 ILE D 104 95.179 59.965 22.895 1.00 17.98 D ATOM 3810 C ILE D 104 95.179 59.965 22.895 1.00 17.98 D ATOM 3811 O ILE D 104 96.887 61.283 17.902 1.00 18.07 D ATOM 3812 N LEU D 105 98.987 60.272 18.509 1.00 16.66 D ATOM 3813 CA LEU D 105 99.370 60.272 18.509 1.00 16.65 D ATOM 3814 CB LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3815 CG LEU D 105 101.864 60.482 16.895 1.00 17.56 D ATOM 3816 CD1 LEU D 105 101.375 61.926 16.842 1.00 21.266 D ATOM 3817 CD2 LEU D 105 100.460 62.771 15.951 1.00 21.266 D ATOM 3819 O LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.368 58.056 18.056 1.00 17.13 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3821 CA ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3821 CA ILE D 106 98.045 57.016 15.839 1.00 17.13 D ATOM 3821 CA ILE D 106 98.045 57.016 15.839 1.00 17.14 D ATOM 3822 CB ILE D 106 96.093 55.496 15.318 1.00 17.14 D ATOM 3824 CG1 ILE D 106 98.045 57.016 15.839 1.00 17.14 D ATOM 3826 C C ILE D 106 98.045 57.016 15.839 1.00 17.14 D ATOM 3827 C CYS D 107 99.540 55.312 14.966 1.00 19.04 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 19.04 D ATOM 3829 CA CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3830 C C CYS D 107 99.635 58.631 1.4.700 1.00 17.19 D ATOM 3831 C C LEU D 108 99.027 53.321 12.493 1.00 17.19 D ATOM 3832 CB CYS D 107 100.339 54.637 13.954 1.00 19.40 D ATOM 3836 CB LEU D 108 99.027 53.321 12.493 1.00 19.40 D ATOM 3837 CG LEU D 108 99.027 53.221 12.493 1.00 19.40 D ATOM 3838 CD LEU D 108 99.027 53.321 12.493 1.00 19.40 D ATOM 3838 CD LEU D 108 99.027 53.221 12.493 1.00 19.40 D ATOM 3838 CD LEU D 108 99.027 53.221 12.493 1.00 19.40 D ATOM 3838 CD LEU D 108 99.027 53.221 12.493 1										
ATOM 3804 N ILE D 104 97.010 62.977 20.284 1.00 17.39 D ATOM 3805 CA ILB D 104 97.465 61.595 20.198 1.00 15.30 D ATOM 3806 CB ILB D 104 96.402 60.627 20.755 1.00 17.89 D ATOM 3807 CG2 ILB D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3808 CG1 ILB D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3808 CG1 ILB D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3808 CG1 ILB D 104 96.818 59.175 20.498 1.00 17.198 D ATOM 3810 C ILB D 104 97.760 61.185 18.763 1.00 17.15 D ATOM 3811 O ILB D 104 97.760 61.185 18.763 1.00 17.15 D ATOM 3811 O ILB D 104 96.887 61.283 17.902 1.00 18.07 D ATOM 3812 N LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3813 CA LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3815 CG LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3815 CG LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3816 CD1 LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3818 C LEU D 105 100.460 62.771 15.951 1.00 21.266 D ATOM 3818 C LEU D 105 100.460 62.771 15.951 1.00 21.266 D ATOM 3818 C LEU D 105 99.368 58.004 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.368 58.004 17.128 1.00 17.13 D ATOM 3820 N ILB D 106 98.432 58.399 16.039 1.00 17.18 D ATOM 3821 CA ILB D 106 98.432 58.399 16.039 1.00 17.18 D ATOM 3822 CB ILB D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3823 CG2 ILB D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3824 CG1 ILB D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3826 C ILB D 106 98.876 56.431 14.700 1.00 17.14 D ATOM 3829 CA CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 99.634 53.323 13.670 1.00 20.08 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.08 D ATOM 3831 C CYS D 107 99.634 53.323 13.670 1.00 20.08 D ATOM 3831 C C CYS D 107 99.635 53.221 12.493 1.00 19.48 D ATOM 3831 C C CYS D 107 100.339 54.637 13.954 1.00 19.48 D ATOM 3831 C C CYS D 107 99.634 53.323 13.670 1.00 20.08 D ATOM 3831 C C CYS D 107 99.635 53.221 12.493 1.00 19.48 D ATOM 3831 C C LEU D 108 99.577 51.358 10.925 1.00 20.40 D ATOM 3831 C C LEU D 108 99.577 51.358 10.925										
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ATOM 3806 CB ILE D 104 96.402 60.627 20.755 1.00 17.89 D ATOM 3807 CG2 ILE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3808 CG1 ILE D 104 96.202 60.886 22.253 1.00 18.46 D ATOM 3809 CD1 ILE D 104 95.179 59.965 22.895 1.00 17.98 D ATOM 3810 C ILE D 104 97.760 61.185 18.763 1.00 17.98 D ATOM 3811 O ILE D 104 96.827 61.283 17.902 1.00 18.07 D ATOM 3811 O ILE D 105 98.987 60.727 18.509 1.00 16.66 D ATOM 3813 CA LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3814 CB LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3815 CG LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3816 CD1 LEU D 105 102.811 61.943 16.302 1.00 21.66 D ATOM 3817 CD2 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3818 C LEU D 105 99.366 58.804 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.368 58.056 18.056 1.00 17.13 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.14 D ATOM 3821 CA ILE D 106 98.432 58.399 15.492 1.00 17.14 D ATOM 3821 CA ILE D 106 96.093 55.496 15.813 1.00 17.14 D ATOM 3822 CB ILE D 106 96.093 55.496 15.318 1.00 17.14 D ATOM 3825 CD1 ILE D 106 98.425 58.999 15.492 1.00 17.14 D ATOM 3826 C ILE D 106 98.876 55.312 14.906 1.00 17.19 D ATOM 3827 O ILE D 106 98.876 55.312 14.906 1.00 17.19 D ATOM 3828 N CYS D 107 99.540 55.312 14.906 1.00 17.19 D ATOM 3829 CA CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3828 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3833 CB CYS D 107 100.339 54.637 13.954 1.00 19.48 D ATOM 3833 CB LEU D 108 99.577 51.358 10.925 1.00 20.40 D ATOM 3833 CC LEU D 108 99.637 53.221 12.493 1.00 19.48 D ATOM 3833 CC LEU D 108 99.637 53.221 12.493 1.00 19.48 D ATOM 3836 CB LEU D 108 99.637 53.231 11.369 1.00 19.44 D	ATOM	3805	CA	ILE I	104	97.465	61.595	20.198	1.00 15.30	D
ATOM 3807 CG2 ILE D 104 96.818 59.175 20.498 1.00 13.27 D ATOM 3808 CG1 ILE D 104 96.202 60.886 22.253 1.00 18.46 ATOM 3809 CD1 ILE D 104 95.179 59.965 22.895 1.00 17.98 D ATOM 3810 C ILE D 104 97.760 61.185 18.763 1.00 17.15 D ATOM 3811 C ILE D 104 96.887 61.283 17.902 1.00 18.07 D ATOM 3812 N LEU D 105 98.987 60.277 18.509 1.00 16.66 D ATOM 3813 CA LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3814 CB LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3815 CG LEU D 105 101.375 61.926 16.842 1.00 21.66 D ATOM 3816 CD1 LEU D 105 102.811 61.943 16.302 1.00 21.26 D ATOM 3817 CD2 LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3818 C LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.368 58.056 18.056 1.00 18.355 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3821 CA ILE D 106 98.045 57.016 15.839 1.00 17.88 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3824 CG1 ILE D 106 99.571 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 99.876 55.312 14.966 1.00 18.05 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 22.00 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 22.00 D ATOM 3832 CB CYS D 107 100.339 54.637 13.954 1.00 19.48 D ATOM 3833 CG LEU D 108 99.075 53.221 12.493 1.00 19.48 D ATOM 3836 CB LEU D 108 99.075 51.358 10.02 19.98 D ATOM 3837 CG LEU D 108 99.075 51.358 10.925 1.00 19.48 D ATOM 3838 CD1 LEU D 108 99.583 51.366 9.412 1.00 20.40 D ATOM 3838 CD1 LEU D 108 99.587 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 99.587 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3831 CA LEU D 108 99.677 51.563 10.170 1.00 20.11 D ATOM 3834 CA VAL D 109 99.677 51.563 10.170 1.00 20.11 D ATOM 3843 CA VAL D 109 99.677 51.565 10.170 1.00 19.64 D		3806	CB	ILR I	104	96.402	60.627	20.755	1.00 17.89	D
ATOM 3808 CGI ILE D 104 96.202 60.886 22.253 1.00 18.46 D ATOM 3809 CDI ILE D 104 95.179 59.965 22.895 1.00 17.98 D ATOM 3810 C ILE D 104 97.760 61.185 18.763 1.00 17.15 D ATOM 3811 O ILE D 104 96.887 61.283 17.902 1.00 18.07 D ATOM 3812 N LEU D 105 98.987 60.727 18.509 1.00 16.66 D ATOM 3813 CA LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3814 CB LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3815 CG LEU D 105 101.375 61.926 16.842 1.00 21.66 D ATOM 3816 CD LEU D 105 100.811 61.943 16.302 1.00 21.66 D ATOM 3817 CD2 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3818 C LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.368 58.056 18.056 1.00 18.35 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.14 D ATOM 3821 CA ILE D 106 96.093 55.496 15.318 1.00 17.14 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.69 D ATOM 3824 CGI ILE D 106 96.093 55.496 15.318 1.00 17.19 D ATOM 3826 C ILE D 106 98.423 57.877 16.260 1.00 18.06 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 15.63 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3831 O CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3833 CG LEU D 108 99.07 53.221 12.493 1.00 19.74 D ATOM 3833 CG LEU D 108 99.07 53.221 12.493 1.00 19.74 D ATOM 3830 C CYS D 107 100.339 54.637 13.954 1.00 19.74 D ATOM 3831 O CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 CG LEU D 108 99.027 53.221 12.493 1.00 19.98 D ATOM 3836 CB LEU D 108 99.027 53.221 12.493 1.00 19.98 D ATOM 3838 CD1 LEU D 108 99.027 53.221 12.493 1.00 19.98 D ATOM 3838 CD1 LEU D 108 99.583 51.366 9.412 1.00 20.15 D ATOM 3838 CD1 LEU D 108 99.587 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 99.587 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 99.587 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 99.630 149.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.657 51.563 10.170 1.00 20.11 D									1.00 13.27	D
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ATOM 3812 N LEU D 105 98.987 60.727 18.509 1.00 16.66 D ATOM 3813 CA LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3814 CB LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3815 CG LEU D 105 101.375 61.926 16.842 1.00 21.66 D ATOM 3816 CD1 LEU D 105 100.864 60.482 16.895 1.00 21.66 D ATOM 3817 CD2 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3818 C LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3821 CA ILE D 106 98.045 57.016 15.839 1.00 17.14 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3823 CG2 ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3825 CD1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3826 C ILE D 106 98.941 57.004 13.618 1.00 17.19 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 17.19 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 16.06 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3828 N CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3833 CG CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3833 CG CYS D 107 99.634 53.323 13.670 1.00 20.08 D ATOM 3833 CG LEU D 108 99.07 53.221 12.493 1.00 19.67 D ATOM 3836 CB LEU D 108 99.07 53.221 12.493 1.00 19.67 D ATOM 3836 CB LEU D 108 99.07 53.221 12.493 1.00 19.67 D ATOM 3836 CB LEU D 108 99.07 53.221 12.493 1.00 19.67 D ATOM 3838 CD1 LEU D 108 99.07 53.221 12.493 1.00 19.67 D ATOM 3838 CD1 LEU D 108 99.07 53.221 12.493 1.00 19.44 D ATOM 3839 CD2 LEU D 108 99.577 51.358 10.925 1.00 20.15 D ATOM 3838 CD1 LEU D 108 99.07 51.358 10.925 1.00 20.15 D ATOM 3840 C LEU D 108 99.07 51.358 10.925 1.00 20.15 D ATOM 3841 O LEU D 108 99.677 51.358 10.925 1.00 20.15 D ATOM 3841 O LEU D 108 99.677 51.358 10.920 1.00 19.44 D ATOM 3841 O LEU D 108 99.677 51.358 10.920 1.00 19.64 D	MOTA	3810	С	ILE I	104	97.760	61.185	18.763	1.00 17.15	D
ATOM 3812 N LEU D 105 98.987 60.727 18.509 1.00 16.66 D ATOM 3813 CA LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3815 CG LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3816 CD1 LEU D 105 101.375 61.926 16.842 1.00 21.66 D ATOM 3816 CD1 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3817 CD2 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3819 O LEU D 105 99.368 55.056 18.056 1.00 18.35 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3821 CA ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3822 CB ILE D 106 96.093 55.496 15.839 1.00 17.14 D ATOM 3823 CG2 ILE D 106 96.093 55.496 15.318 1.00 15.63 D ATOM 3825 CD1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 17.19 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 17.19 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3820 CB ILE D 106 98.941 57.004 13.618 1.00 17.19 D ATOM 3820 CB CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3833 CG CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3834 N LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3838 CD LEU D 108 99.027 53.221 12.493 1.00 19.67 D ATOM 3838 CD LEU D 108 99.027 53.221 12.493 1.00 19.67 D ATOM 3838 CD LEU D 108 99.027 53.521 12.493 1.00 19.48 D ATOM 3838 CD LEU D 108 99.027 53.521 12.493 1.00 19.48 D ATOM 3839 CD LEU D 108 99.027 53.521 12.493 1.00 19.44 D ATOM 3834 CA LEU D 108 99.577 51.358 10.925 1.00 20.15 D ATOM 3834 CA LEU D 108 99.027 51.355 10.170 1.00 20.15 D ATOM 3834 CA LEU D 108 99.027 51.355 10.170 1.00 20.15 D ATOM 3834 CA LEU D 108 99.027 51.355 10.170 1.00 20.15 D ATOM 3834 CA LEU D 108 99.027 51.355 10.170 1.00 20.11 D ATOM 3842 CA LEU D 108 99.027 51.355 10.170 1.00 20.11 D ATOM 3844 CA LEU D 108 99.027 51.355 10.170 1.00 20.11 D ATOM 3844 CA LEU D 108 99.027 51.355 10.170 1.00 2	ATOM	3811	0	ILE I	104	96.887	61.283	17.902	1.00 18.07	D
ATOM 3813 CA LEU D 105 99.370 60.272 17.177 1.00 16.59 D ATOM 3814 CB LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3815 CG LEU D 105 101.375 61.926 16.895 1.00 21.266 D ATOM 3816 CD1 LEU D 105 102.811 61.943 16.302 1.00 21.26 D ATOM 3817 CD2 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3818 C LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.368 58.056 18.056 1.00 18.35 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3821 CA ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3823 CG2 ILE D 106 96.093 55.496 15.318 1.00 15.63 D ATOM 3824 CG1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 98.876 56.431 14.700 1.00 16.48 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 16.06 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3833 CB CYS D 107 100.339 54.637 13.954 1.00 19.74 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.67 D ATOM 3835 CA LEU D 108 99.027 53.221 12.493 1.00 19.67 D ATOM 3836 CB LEU D 108 99.027 53.221 12.493 1.00 19.67 D ATOM 3837 CG LEU D 108 99.027 53.221 12.493 1.00 19.67 D ATOM 3838 CD LEU D 108 99.027 53.221 12.493 1.00 19.67 D ATOM 3838 CD LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3839 CD2 LEU D 108 99.027 51.258 11.369 1.00 19.48 D ATOM 3839 CD2 LEU D 108 99.027 51.258 10.22 1.00 20.15 D ATOM 3834 CA LEU D 108 99.027 51.258 10.237 10.00 20.15 D ATOM 3839 CD2 LEU D 108 99.027 51.145 11.364 1.00 19.44 D ATOM 3841 O LEU D 108 99.027 51.145 11.367 1.00 20.15 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.64 D						98.987	60.727	18,509	1.00 16.66	Ð
ATOM 3814 CB LEU D 105 100.864 60.482 16.895 1.00 17.56 D ATOM 3815 CG LEU D 105 101.375 61.926 16.842 1.00 21.66 D ATOM 3816 CD1 LEU D 105 102.811 61.943 16.302 1.00 21.26 D ATOM 3817 CD2 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3818 C LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.368 58.056 18.056 1.00 18.35 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3821 CA ILE D 106 98.045 57.016 15.839 1.00 17.14 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3823 CG2 ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3824 CG1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 98.876 56.431 14.700 19.04 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 10.0 17.19 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 16.06 D ATOM 3829 CA CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3833 CB CYS D 107 100.339 54.637 13.954 1.00 19.74 D ATOM 3834 N LEU D 108 99.037 53.221 12.493 1.00 22.00 D ATOM 3833 CB CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3836 CB LEU D 108 99.027 53.221 12.493 1.00 19.98 D ATOM 3837 CG LEU D 108 99.027 53.221 12.493 1.00 19.98 D ATOM 3838 CD LEU D 108 99.027 51.358 10.925 1.00 20.40 D ATOM 3839 CD LEU D 108 99.027 51.358 10.925 1.00 20.40 D ATOM 3839 CD LEU D 108 99.027 51.358 10.925 1.00 20.40 D ATOM 3839 CD LEU D 108 99.027 51.358 10.925 1.00 20.40 D ATOM 3830 CD LEU D 108 99.027 51.358 10.925 1.00 20.40 D ATOM 3831 CD LEU D 108 99.027 51.358 10.925 1.00 19.98 D ATOM 3834 N LEU D 108 99.027 51.358 10.925 1.00 20.40 D ATOM 3836 CD LEU D 108 99.027 51.358 10.925 1.00 20.40 D ATOM 3837 CG LEU D 108 99.027 51.358 10.925 1.00 20.40 D ATOM 3838 CD LEU D 108 99.027 51.358 10.925 1.00 20.40 D ATOM 3834 N VAL D 109 99.473 49.940 11.721 1.00 19.64 D										D
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ATOM 3816 CD1 LEU D 105 102.811 61.943 16.302 1.00 21.26 D ATOM 3817 CD2 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3818 C LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.368 58.056 18.056 1.00 18.35 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3821 CA ILE D 106 96.432 58.399 15.492 1.00 17.14 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3823 CG2 ILE D 106 96.093 55.496 15.318 1.00 15.63 D ATOM 3824 CG1 ILE D 106 94.238 57.877 16.260 1.00 19.04 D ATOM 3825 CD ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 16.06 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 19.74 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3833 CG CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3837 CG LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3838 CD LEU D 108 99.027 53.221 12.493 1.00 19.98 D ATOM 3839 CD LEU D 108 99.027 51.358 10.925 1.00 20.40 D ATOM 3838 CD LEU D 108 99.075 51.358 10.925 1.00 20.40 D ATOM 3830 CD LEU D 108 99.077 51.358 10.925 1.00 20.40 D ATOM 3831 CD LEU D 108 99.077 51.358 10.925 1.00 20.40 D ATOM 3834 N VAL D 109 99.473 49.940 11.721 1.00 19.64 D	MOTA	3814								
ATOM 3817 CD2 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3818 C LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.368 58.056 18.056 1.00 18.35 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.18 D ATOM 3821 CA ILE D 106 96.525 56.939 15.492 1.00 17.14 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3823 CG2 ILE D 106 96.093 55.496 15.318 1.00 15.63 D ATOM 3824 CG1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 94.238 57.877 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 16.06 D ATOM 3829 CA CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3833 CG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.48 D ATOM 3836 CB LEU D 108 98.313 52.015 12.113 1.00 19.49 D ATOM 3837 CG LEU D 108 99.027 53.221 12.493 1.00 19.49 D ATOM 3838 CD1 LEU D 108 99.583 51.366 9.412 1.00 19.49 D ATOM 3838 CD1 LEU D 108 99.583 51.366 9.412 1.00 19.49 D ATOM 3838 CD1 LEU D 108 99.583 51.366 9.412 1.00 19.49 D ATOM 3834 C LEU D 108 99.677 51.358 10.925 1.00 20.40 D ATOM 3834 C LEU D 108 99.583 51.366 9.412 1.00 19.49 D ATOM 3836 CD LEU D 108 99.583 51.366 9.412 1.00 19.49 D ATOM 3836 CD LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 19.64 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 19.64 D	MOTA	3815	CG	LEU I	105	101.375	61.926	16.842	1.00 21.66	D
ATOM 3817 CD2 LEU D 105 100.460 62.771 15.951 1.00 21.56 D ATOM 3818 C LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.368 58.056 18.056 1.00 18.35 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3821 CA ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3823 CG2 ILE D 106 96.093 55.496 15.318 1.00 15.63 D ATOM 3824 CG1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 94.238 57.877 16.260 1.00 16.48 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 16.06 D ATOM 3829 CA CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3830 C CYS D 107 99.632 52.421 14.507 1.00 20.17 D ATOM 3831 O CYS D 107 99.632 52.421 14.507 1.00 20.17 D ATOM 3831 O CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 CG LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3836 CD LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3837 CG LEU D 108 99.583 51.366 9.412 1.00 19.48 D ATOM 3838 CD LEU D 108 99.583 51.366 9.412 1.00 19.48 D ATOM 3838 CD LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD LEU D 108 99.583 51.366 9.412 1.00 19.48 D ATOM 3838 CD LEU D 108 99.631 42.351 11.369 1.00 19.48 D ATOM 3838 CD LEU D 108 99.583 51.366 9.412 1.00 19.48 D ATOM 3838 CD LEU D 108 99.657 51.553 10.170 1.00 20.15 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 19.32 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 19.32 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 19.32 D ATOM 3843 CA VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 99.473 49.940 11.721 1.00 19.32	MOTA	3816	CD1	LEU I	105	102.811	61.943	16.302	1.00 21.26	D
ATOM 3818 C LEU D 105 99.061 58.804 17.128 1.00 17.13 D ATOM 3819 O LEU D 105 99.368 58.056 18.056 1.00 18.35 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.18 D ATOM 3821 CA ILE D 106 98.045 57.016 15.839 1.00 17.14 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3823 CG2 ILE D 106 96.093 55.496 15.318 1.00 15.63 D ATOM 3824 CG1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 94.238 57.877 16.260 1.00 16.48 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3832 CB CYS D 107 100.339 54.637 13.954 1.00 19.74 D ATOM 3833 CG CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.67 D ATOM 3835 CA LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3836 CB LEU D 108 99.027 53.221 12.493 1.00 19.67 D ATOM 3837 CG LEU D 108 99.313 52.015 12.113 1.00 19.67 D ATOM 3838 CD1 LEU D 108 99.313 52.015 12.113 1.00 19.67 D ATOM 3837 CG LEU D 108 99.027 53.221 12.493 1.00 19.98 D ATOM 3838 CD1 LEU D 108 99.5977 51.358 10.925 1.00 20.40 D ATOM 3839 CD2 LEU D 108 99.007 51.145 11.237 1.00 19.44 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.677 51.145 11.237 1.00 19.44 D ATOM 3841 O LEU D 108 99.677 51.145 11.237 1.00 19.44 D ATOM 3841 O LEU D 108 99.677 51.145 11.237 1.00 19.44 D ATOM 3841 O LEU D 108 99.677 51.145 11.237 1.00 19.44 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D									1.00 21.56	D
ATOM 3819 O LEU D 105 99.368 58.056 18.056 1.00 18.35 D ATOM 3820 N ILE D 106 98.432 58.399 16.039 1.00 17.88 D ATOM 3821 CA ILE D 106 98.045 57.016 15.839 1.00 17.14 D ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3823 CG2 ILE D 106 96.093 55.496 15.318 1.00 15.63 D ATOM 3824 CG1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 94.238 57.877 16.260 1.00 16.48 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 16.06 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3832 CB CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 SG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 CG LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 99.207 51.358 10.925 1.00 20.40 D ATOM 3834 N LEU D 108 99.577 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 99.207 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 99.577 51.358 10.925 1.00 19.48 D ATOM 3838 CD1 LEU D 108 99.657 51.358 10.925 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D										
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ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3823 CG2 ILE D 106 96.093 55.496 15.318 1.00 15.63 D ATOM 3824 CG1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 94.238 57.877 16.260 1.00 16.48 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 16.06 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 99.634 55.312 14.966 1.00 18.84 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3832 CB CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3833 SG CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 CG LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3838 CD1 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3834 O LEU D 108 99.07 51.145 11.237 1.00 19.44 D ATOM 3840 C LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.64 D	ATOM	3820	N	ILE I	D 106	98.432	58.399	16.039	1.00 17.88	D
ATOM 3822 CB ILE D 106 96.525 56.939 15.492 1.00 16.99 D ATOM 3823 CG2 ILE D 106 96.093 55.496 15.318 1.00 15.63 D ATOM 3824 CG1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 94.238 57.877 16.260 1.00 16.48 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 16.06 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 99.634 53.323 13.670 1.00 19.74 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3832 CB CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 SG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3835 CA LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3836 CB LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3834 C LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3834 C LEU D 108 99.07 51.145 11.237 1.00 19.44 D ATOM 3834 C LEU D 108 99.207 51.145 11.237 1.00 19.44 D ATOM 3834 C LEU D 108 99.207 51.145 11.237 1.00 19.44 D ATOM 3840 C LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D	MOTA	3821	CA	ILE 1	0 106	98.045	57.016	15.839	1.00 17.14	D
ATOM 3823 CG2 ILE D 106 96.093 55.496 15.318 1.00 15.63 D ATOM 3824 CG1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 94.238 57.877 16.260 1.00 16.48 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 16.06 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 100.339 54.637 13.954 1.00 19.74 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3832 CB CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 SG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3830 C LEU D 108 99.075 51.358 10.925 1.00 20.15 D ATOM 3834 O LEU D 108 99.207 55.125 12.113 1.00 19.48 D ATOM 3838 CD1 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.64 D						96.525	56.939	15.492	1.00 16.99	D
ATOM 3824 CG1 ILE D 106 95.711 57.619 16.604 1.00 19.04 D ATOM 3825 CD1 ILE D 106 94.238 57.877 16.260 1.00 16.48 D ATOM 3826 C ILE D 106 98.876 56.431 14.700 1.00 17.19 D ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 16.06 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 100.339 54.637 13.954 1.00 19.74 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3832 CB CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3833 SG CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 SG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3835 CA LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 99.473 49.940 11.721 1.00 19.32 D										D
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ATOM 3827 O ILE D 106 98.941 57.004 13.618 1.00 16.06 D ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 100.339 54.637 13.954 1.00 19.74 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3832 CB CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 SG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.44 D ATOM 3841 O LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64			C	ILE :	D 106	98.876	56.431	14.700	1.00 17.19	D
ATOM 3828 N CYS D 107 99.540 55.312 14.966 1.00 18.84 D ATOM 3829 CA CYS D 107 100.339 54.637 13.954 1.00 19.74 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3832 CB CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 SG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 20.11 D ATOM 3843 CA VAL D 109 99.473 49.940 11.721 1.00 19.32 D								13.618		D
ATOM 3829 CA CYS D 107 100.339 54.637 13.954 1.00 19.74 D ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3832 CB CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 SG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.67 D ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.44 D ATOM 3841 O LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64										
ATOM 3830 C CYS D 107 99.634 53.323 13.670 1.00 20.17 D ATOM 3831 O CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3832 CB CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 SG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.44 D ATOM 3841 O LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64										
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ATOM 3831 O CYS D 107 99.632 52.421 14.507 1.00 20.08 D ATOM 3832 CB CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 SG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64	ATOM	3830	С	CYS	D 107	99.634	53.323	13.670	1.00 20.17	D
ATOM 3832 CB CYS D 107 101.755 54.349 14.453 1.00 22.00 D ATOM 3833 SG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64	MOTA	3831	0	CYS	D 107	99.632	52.421	14.507	1.00 20.08	D
ATOM 3833 SG CYS D 107 102.800 53.514 13.211 1.00 28.61 D ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64										ם
ATOM 3834 N LEU D 108 99.027 53.221 12.493 1.00 19.48 D ATOM 3835 CA LEU D 108 98.313 52.015 12.113 1.00 19.67 D ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 C3 LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64										
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ATOM 3836 CB LEU D 108 97.024 52.391 11.369 1.00 19.98 D ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64 D	MOTA	3835	CA	LEU	D 108	98.313	52.015	12.113		
ATOM 3837 CG LEU D 108 95.977 51.358 10.925 1.00 20.40 D ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64 D			CB	LEU	D 108	97.024	52.391	11.369	1.00 19.98	D
ATOM 3838 CD1 LEU D 108 95.883 51.366 9.412 1.00 20.15 D ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64 D									1.00 20.40	D
ATOM 3839 CD2 LEU D 108 96.301 49.971 11.454 1.00 19.44 D ATOM 3840 C LEU D 108 99.207 51.145 11.237 1.00 19.84 D ATOM 3841 O LEU D 108 99.657 51.563 10.170 1.00 20.11 D ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64 D										
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ATOM 3842 N VAL D 109 99.473 49.940 11.721 1.00 19.32 D ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64 D	MOTA	3841	0	LEU	D 108	99.657		10.170		
ATOM 3843 CA VAL D 109 100.289 48.972 11.016 1.00 19.64 D	ATOM		N	VAL	D 109	99.473	49.940	11.721	1.00 19.32	D
Alon Joly Ca van D 200										D

MOTA	3844	CB	VAL D 10:	101.368	48.402	11.958	1.00 19.40	D
ATOM	3845		VAL D 10		47.474	11.202	1.00 18.01	ם
ATOM	3846		VAL D 10		49.560	12.590	1.00 17.30	D
ATOM	3847	C	VAL D 10		47.876	10.568	1.00 21.45	D
ATOM ATOM	3848 3849	O N	VAL D 10 ASP D 11		47.079 47.861	11.382 9.274	1.00 22.65 1.00 22.00	D D
ATOM	3850	CA	ASP D 11			8.689	1.00 23.80	Ď
ATOM	3851	CB	ASP D 11			7.728	1.00 24.68	D
ATOM	3852	CG	ASP D 11			7.603	1.00 26.64	D
MOTA	3853		ASP D 11			8.177	1.00 28.80	D
ATOM	3854	OD2	ASP D 11	0 94.920	47.591	6.926	1.00 27.99	D
ATOM	3855	C	ASP D 11			7.944	1.00 23.77	D
MOTA	3856	0	ASP D 11			7.684	1.00 22.82	D
ATOM	3857	N	ASN D 11			7.604	1.00 23.55	D
MOTA	3858	CA	ASN D 11 ASN D 11			6.889 5.425	1.00 23.79 1.00 25.36	D D
MOTA MOTA	3859 3860	CB CG	ASN D 11			4.562	1.00 29.95	D
ATOM	3861		ASN D 11			3.724	1.00 29.58	D
ATOM	3862		ASN D 11			4.761	1.00 30.51	D
ATOM	3863	C	ASN D 11	1 99.786	42.941	7.556	1.00 22.70	D
MOTA	3864	0	ASN D 11	1 100.834	42.784	6.929	1.00 22.97	D
MOTA	3865	N	ILE D 11			8.835	1.00 22.14	D
ATOM	3866	CA	ILE D 11			9.598	1.00 20.20	D
ATOM	3867	СВ	ILE D 11			11.055	1.00 18.82 1.00 15.77	D D
ATOM	3868	CG2 CG1	ILE D 11			11.808 11.103	1.00 15.77	ם
ATOM ATOM	3869 3870		ILE D 11			12.514	1.00 21.18	D
ATOM	3871	C	ILE D 11			9.659	1.00 21.41	D
ATOM	3872	ō	ILE D 11			10.002	1.00 22.04	D
ATOM	3873	N	PHE D 11	3 101.765	39.838	9.338	1.00 21.35	D
ATOM	3874	CA	PHE D 11			9.409	1.00 19.93	D
ATOM	3875	CB	PHE D 11			8.462	1.00 21.28	D
ATOM	3876	CG	PHE D 11			8.825	1.00 20.91	D D
ATOM	3877		PHE D 11			9.838 8.230	1.00 19.85 1.00 22.61	D
ATOM ATOM	3878 3879		PHE D 11			10.264	1.00 20.63	D
ATOM	3880	CE2				8.646	1.00 21.21	D
ATOM	3881	CZ	PHE D 11			9.669	1.00 20.87	D
MOTA	3882	С	PHE D 11	3 103.201	37.871	9.071	1.00 19.98	D
MOTA	3883	0	PHE D 11	3 103.762		8.044	1.00 20.80	D
MOTA	3884	N	PRO D 11			9.925	1.00 21.26	D
ATOM	3885	CD.	PRO D 11			9.732	1.00 21.94	D D
MOTA	3886 3887	CA CB	PRO D 11			11.166 11.625	1.00 21.41 1.00 21.03	D
MOTA MOTA	3888	CG	PRO D 11			11.115	1.00 22.98	D
ATOM	3889	c	PRO D 11			12.185	1.00 21.84	ם
ATOM	3890	0	PRO D 11	4 103.621	38.711	12.034	1.00 20.41	Ð
MOTA	3891	N	PRO D 11			13.222	1.00 22.52	D
ATOM	3892	CD	PRO D 11			13.445	1.00 22.08	D
MOTA	3893	CA	PRO D 11			14.266	1.00 21.19	D D
ATOM	3894	CB	PRO D 11			15.025 14.902	1.00 20.92 1.00 19.88	ם
ATOM ATOM	3895 3896	CG C	PRO D 11			15.171	1.00 21.62	D
ATOM	3897	Ö	PRO D 13			16.356	1.00 22.92	D
ATOM	3898	N	VAL D 1			14.588	1.00 21.58	a
MOTA	3899	CA	VAL D 1	.6 105.409	39.598	15.300	1.00 22.53	D
MOTA	3900	СВ	VAL D 1			15.067	1.00 24.90	Ď
MOTA	3901		VAL D 1			15.713	1.00 24.06	D
ATOM	3902		VAL D 1			15.641	1.00 24.88	. D
MOTA	3903	C	VAL D 1			14.708 13.509	1.00 21.86 1.00 20.87	D
ATOM ATOM	3904 3905	Ŋ	VAL D 1: VAL D 1:			15.534	1.00 20.65	D
MOTA	3906	CA	VAL D 1			15.007	1.00 21.60	D
MOTA	3907	CB	VAL D 1	-			1.00 18.11	D
ATOM	3908	CG1	VAL D 1	104.15	6 44.473	15.403	1.00 16.63	D
MOTA	3909		VAL D 1				1.00 17.02	D
MOTA	3910	С	VAL D 1				1.00 23.84	Q Q
ATOM	3911	0	VAL D 1				1.00 24.78	D D
ATOM	3912	N	ASN D 1				1.00 27.93 1.00 30.45	D
MOTA MOTA	3913 3914	CA CB	ASN D 1				1.00 30.45	D
ATOM	3914	CG	ASN D 1				1.00 39.88	ם
MOTA	3916		LASN D 1				1.00 42.45	D
MOTA	3917		ASN D 1				1.00 43.14	D

ATOM	3918	C	ASN D 118	107.960	47.465	16.181	1.00 27.72	D
MOTA	3919	0	ASN D 118	108.398	47.952	15.140	1.00 26.88	D
ATOM	3920	N	ILE D 119	107.126	48.113	16.988 16.700	1.00 27.59 1.00 27.12	D D
ATOM ATOM	3921 3922	CA CB	ILE D 119 ILE D 119	106.680 105.133	49.476 49.580	16.700	1.00 27.12	D
ATOM	3923		ILE D 119	104.698	50.994	16.346	1.00 26.16	D
ATOM	3924		ILE D 119	104.528	48.572	15.741	1.00 24.63	D
ATOM	3925	CD1	ILE D 119	103.026	48.423	15.877	1.00 24.19	D
MOTA	3926	C	ILE D 119	107.243	50.436	17.746	1.00 27.72	D
ATOM	3927	0	ILE D 119	107.050	50.248	18.946	1.00 26.86	D
MOTA	3928	N	THR D 120 THR D 120	107.951 108.524	51.460 52.423	17.291 18.214	1.00 27.54 1.00 29.37	D D
MOTA MOTA	3929 3930	CA CB	THR D 120	110.022	52.131	18.477	1.00 32.22	ā
ATOM	3931		THR D 120	110.722	52.034	17.229	1.00 35.14	D
ATOM	3932	CG2	THR D 120	110.176	50.817	19.247	1.00 35.67	D
ATOM	3933	C	THR D 120	108.369	53.826	17.668	1.00 27.95	D
ATOM	3934	0	THR D 120	108.398	54.035	16.459	1.00 29.89 1.00 26.28	D D
ATOM	3935	N CA	TRP D 121 TRP D 121	108.187 108.031	54.789 56.171	18.560 18.135	1.00 26.23	ď
ATOM ATOM	3936 3937	CB	TRP D 121	106.935	56.866	18.940	1.00 24.20	D
ATOM	3938	CG	TRP D 121	105.568	56.343	18.687	1.00 22.03	D
ATOM	3939	CD2	TRP D 121	104.643	56.826	17.707	1.00 20.30	D
MOTA	3940	CE2		103.454	56.085	17.856	1.00 20.70	D
MOTA	3941		TRP D 121	104.705	57.817	16.717	1.00 17.15	D D
ATOM	3942		TRP D 121	104.929 103.655	55.351 55.190	19.365 18.875	1.00 21.06 1.00 22.39	D
MOTA MOTA	3943 3944		TRP D 121	102.332	56.305	17.057	1.00 17.25	D
ATOM	3945	CZ3		103.593	58.036	15.924	1.00 17.92	D
MOTA	3946		TRP D 121	102.419	57.282	16.099	1.00 19.11	Ø
MOTA	3947	C	TRP D 121	109.319	56.957	18.284	1.00 26.88	D
MOTA	3948	0	TRP D 121	110.059	56.789	19.251	1.00 27.48 1.00 29.82	D D
ATOM	3949	N CA	LEU D 122 LEU D 122	109.572 110.764	57.830 58.658	17.321 17.343	1.00 23.82	D
MOTA MOTA	3950 3951	CB	LEU D 122	111.664	58.331	16.144	1.00 34.65	D
ATOM	3952	CG	LEU D 122	112.391	56.977	16.112	1.00 37.28	D
ATOM	3953		LEU D 122	113.247	56.828	17.360	1.00 37.11	D
ATOM	3954		LEU D 122	111.394	55.840	16.025	1.00 39.41	ם ס
ATOM	3955	C	LEU D 122	110.416 109.619	60.142 60.593	17.324 16.503	1.00 31.97 1.00 31.46	D
ATOM ATOM	3956 3957	И	LEU D 122 SER D 123	111.010	60.889	18.250	1.00 31.03	D
MOTA	3958	CA	SER D 123	110.813	62.331	18.326	1.00 33.04	D
ATOM	3959	CB	SER D 123	110.312	62.745	19.712	1.00 32.42	D
MOTA	3960	OG	SER D 123	110.169	64.154	19.793	1.00 32.43	D
ATOM	3961	C	SER D 123	112.184	62.948 62.784	18.062 18.860	1.00 33.10 1.00 33.57	D D
ATOM ATOM	3962 3963	o N	SER D 123 ASN D 124	113.108 112.309	63.646	16.941	1.00 33.51	D
ATOM	3964	CA	ASN D 124	113.575	64.258	16.553	1.00 36.20	D
MOTA	3965	CB	ASN D 124	113.963	65.392	17.510	1.00 34.61	D
MOTA	3966	CG	ASN D 124	112.946	66.512	17.531	1.00 34.17	D
ATOM	3967		L ASN D 124	112.262	66.764	16.539	1.00 34.73 1.00 35.34	D D
ATOM	3968	_	ASN D 124 ASN D 124	112.850 114.664	67.202 63.191	18.660 16.561	1.00 37.34	D
MOTA MOTA	3969 3970	0	ASN D 124	115.747	63.401	17.104	1.00 37.93	D
ATOM	3971	N	GLY D 125	114.358	62.039	15.970	1.00 38.73	D
MOTA	3972	CA	GLY D 125	115.317	60.951	15.910	1.00 39.56	D
MOTA	3973	С	GLY D 125	115.457	60.131	17.183	1.00 40.55	D D
ATOM	3974	0	GLY D 125	116.051 114.911	59.054 60.622	17.157 18.291	1.00 42.52 1.00 40.35	D
MOTA MOTA	3975 3976	N CA	HIS D 126	115.009	59.918	19.569	1.00 41.15	D
ATOM	3977	CB	_	115.234	60.923	20.702	1.00 43.51	. Д
ATOM	3978	CG		116.525	61.678	20.599	1.00 47.67	D
ATOM	3979	CD	2 HIS D 126	116.775	62.997	20.422	1.00 47.36	D
MOTA	3980		1 HIS D 126	117.757	61.064	20.694	1.00 49.39	D D
ATOM	3981		1 HIS D 126	118.709 118.140	61.973 63.154	20.581	1.00 48.59 1.00 48.17	D
MOTA MOTA	3982 3983		2 HIS D 126 HIS D 126	113.794	59.053	19.907	1.00 40.38	D
ATOM	3984		HIS D 126	112.648	59.458	19.706	1.00 39.87	D
ATOM	3985		SER D 127	114.056	57.863	20.438	1.00 39.11	D
MOTA	3986			112.995	56.939	20.821	1.00 39.54	ם a
MOTA	3987			113.592 114.299	55.592 55.001	21.232 20.159	1.00 40.04 1.00 45.08	ם
MOTA MOTA	3988 3989		SER D 127 SER D 127	112.167	57.492	21.979	1.00 38.18	D
ATOM	3990		SER D 127	112.707	58.054	22.930	1.00 38.52	D
ATOM	3991		VAL D 128	110.854	57.326	21.894	1.00 36.40	D

MOTA	3992	CA	VAL D 128	109.967	57.800	22.942	1.00 35.00	D
MOTA	3993	CB	VAL D 128	108.699	58.444	22.358	1.00 33.68	D
MOTA	3994	CG1	VAL D 128	107.834	59.001	23.479	1.00 32.31	D
MOTA	3995	CG2	VAL D 128	109.081	59.543	21.383	1.00 32.69	D
MOTA	3996	C	VAL D 128	109.574	56.608	23.790	1.00 34.62	D
MOTA	3997	0	VAL D 128	109.150	55.584	23.268	1.00 35.98	D
ATOM	3998	N	THR D 129	109.715	56.743	25.100	1.00 35.57	D
MOTA	3999	CA	THR D 129	109.393	55.653	26.007	1.00 38.21	D
ATOM	4000	CB	THR D 129	110.562	55.410	26.992	1.00 40.63	D
ATOM	4001	OG1	THR D 129	110.184	54.413	27.949	1.00 44.78	D
ATOM	4002	CG2	THR D 129	110.929	56.700	27.715	1.00 42.66	D
ATOM	4003	С	THR D 129	108.103	55.862	26.799	1.00 36.54	D
ATOM	4004	0	THR D 129	107.359	54.911	27.042	1.00 38.87	D
ATOM	4005	N	GLU D 130	107.833	57.101	27.195	1.00 33.00	D
ATOM	4006	CA	GLU D 130	106.631	57.401	27.963	1.00 31.03	D
ATOM	4007	СВ	GLU D 130	106.935	58.453	29.039	1.00 33.90	D
ATOM	4008	CG	GLU D 130	108.067	58.089	29.987	1.00 38.08	D
ATOM	4009	CD	GLU D 130	107.809	56.788	30.731	1.00 43.43	Ø
ATOM	4010		GLU D 130	106.744	56.672	31.375	1.00 45.61	D
ATOM	4011		GLU D 130	108.671	55.879	30.675	1.00 45.67	D
ATOM	4012	C	GLU D 130	105.521	57.922	27.058	1.00 27.87	D
ATOM	4013	Ö	GLU D 130	105.795	58.527	26.029	1.00 24.56	D
	4014	N	GLY D 131	104.272	57.692	27.457	1.00 26.29	ם
MOTA			GLY D 131	103.140	58.166	26.679	1.00 25.19	D
MOTA	4015	CA	GLY D 131	102.826	57.304	25.474	1.00 24.46	D
MOTA	4016	C	GLY D 131		57.725	24.559	1.00 23.65	D
MOTA	4017	0	VAL D 132	102.130 103.349	56.089	25.476	1.00 22.83	D
MOTA	4018	N	VAL D 132	103.117	55.169	24.379	1.00 23.04	D
ATOM	4019	CA		104.448	54.674	23.784	1.00 22.91	D
ATOM	4020	CB	VAL D 132		53.538	22.821	1.00 24.12	D
MOTA	4021		VAL D 132	104.182	55.816	23.076	1.00 22.85	D
ATOM	4022	CG2		105.164			1.00 21.91	Ď
ATOM	4023	C	VAL D 132	102.326	53.943	24.829 25.917	1.00 21.31	D
MOTA	4024	0	VAL D 132	102.535	53.416		1.00 22.08	Ď
MOTA	4025	N	SER D 133	101.412	53.499	23.979	1.00 22.05	D
MOTA	4026	CA	SER D 133	100.622	52.307	24.251		D
ATOM	4027	CB	SER D 133	99.405	52.637	25.119	1.00 21.95	
ATOM	4028	OG	SER D 133	98.567	53.595	24.498	1.00 27.01	D
MOTA	4029	C	SER D 133	100.178	51.738	22.908	1.00 21.27	D
ATOM	4030	0	SER D 133	100.344	52.369	21.864	1.00 19.82	D
ATOM	4031	N	GLU D 134	99.627	50.538	22.926	1.00 20.29	D
MOTA	4032	CA	GLU D 134	99.182	49.938	21.689	1.00 24.12	D
MOTA	4033	CB	GLU D 134	100.370	49.323	20.932	1.00 26.01	D
ATOM	4034	CG	GLU D 134	100.932	48.045	21.532	1.00 30.80	D
MOTA	4035	CD	GLU D 134	102.080	47.480	20.704	1.00 35.43	D
MOTA	4036		GLU D 134	102.273	46.243	20.702	1.00 36.93	D
MOTA	4037	OE2	GLU D 134	102.793	48.278	20.057	1.00 37.66	D
MOTA	4038	C	GLU D 134	98.127	48.882	21.955	1.00 22.81	D
ATOM	4039	0	GLU D 134	97.968	48.416	23.081	1.00 22.94	D
MOTA	4040	N	THR D 135	97.400	48.522	20.908	1.00 21.95	D
ATOM	4041	CA	THR D 135	96.361	47.519	21.009	1.00 20.78	D
ATOM	4042	CB	THR D 135	95.368	47.625	19.843	1.00 20.82	D
ATOM	4043	OG		96.032	47.262	18.623	1.00 22.24	D
ATOM	4044	CG	2 THR D 135	94.833	49.046	19.721	1.00 18.01	D
MOTA	4045	С	THR D 135	97.037	46.168	20.890	1.00 20.80	D
MOTA	4046	0	THR D 135	98.259	46.084	20.742	1.00 21.08	D
ATOM	4047	N	SER D 136	96.234	45.116	20.972	1.00 19.11	D
ATOM	4048	CA	SER D 136	96.728	43.764	20.790	1.00 16.93	D
MOTA	4049	CB	SER D 136	95.769	42.755	21.428	1.00 19.17	D
ATOM	4050	OG	SER D 136	95.656	42.951	22.831	1.00 23.01	D
ATOM	4051	C	SER D 136	96.665	43.635	19.267	1.00 15.30	D
ATOM	4052	0	SER D 136	96.325	44.592	18.580	1.00 13.19	D
ATOM	4053	N	PHE D 137	97.002	42.472	18.733	1.00 16.43	D
ATOM	4054	CA	PHE D 137	96.896	42.267	17.294	1.00 16.20	D
ATOM	4055	СВ		97.652	41.001	16.874	1.00 15.86	D
ATOM	4056	CG		99.138	41.146	16.879	1.00 17.29	Ð
ATOM	4057		1 PHE D 137	99.792	41.775	15.823	1.00 20.23	D
ATOM	4058		2 PHB D 137	99.894	40.644	17.932	1.00 17.79	D
MOTA	4059		1 PHE D 137	101.187	41.900	15.815	1.00 21.20	D
ATOM	4060		2 PHE D 137	101.291	40.762	17.936		D
ATOM	4061			101.935	41.392	16.874	1.00 19.70	D
ATOM	4062		PHE D 137	95.402	42.056	17.025		D
MOTA	4062		PHE D 137	94.823	41.121	17.556		D
MOTA	4064		LEU D 138	94.786	42.925	16.227		D
MOTA	4065			93.367				D
AT ON	4000	_ un			•			

7.004		~	7 77 T 170	92.722	44.175	15.678	1.00 21.40	D
ATOM	4066	CB	TEO D 138					
ATOM	4067	CG	LEU D 138	92.452	45.087	16.881	1.00 22.42	D
ATOM	4068	CDI	LEU D 138	91.889	44.277	.18.032	1.00 23.38	D
ATOM	4069	CD2	LEU D 138	93.732	45.764	17.301	1.00 28.68	D
ATOM	4070	C	LEU D 138	93.230	41.982	14.593	1.00 20.56	D
ATOM	4071	0	LEU D 138	93.919	42.244	13.615	1.00 22.27	D
	4072	N	SER D 139	92.326	41.013	14.586	1.00 20.44	D
MOTA							1.00 19.23	D
ATOM	4073	CA	SER D 139	92.143	40.142	13.427		
ATOM	4074	CB	SER D 139	91.222	38.986	13.788	1.00 19.74	D
MOTA	4075	OG	SER D 139	89.888	39.443	13.861	1.00 21.32	D
ATOM	4076	C	SER D 139	91.594	40.802	12.168	1.00 19.43	D,
ATOM	4077	ō	SER D 139	91.028	41.893	12.210	1.00 19.49	D
			LYS D 140	91.755	40.102	11.050	1.00 18.62	D
ATOM	4078	N						Ď
ATOM	4079	CA	LYS D 140	91.276	40.553	9.749	1.00 19.20	
MOTA	4080	CB	LYS D 140	92.437	41.058	8.895	1.00 18.92	D
MOTA	4081	CG	LYS D 140	93.286	42.126	9.554	1.00 19.38	D
MOTA	4082	CD	LYS D 140	93.254	43.393	8.758	1.00 20.95	D
ATOM	4083	CE	LYS D 140	93.833	43.195	7.377	1.00 18.23	D
				93.743	44.457	6.617	1.00 20.40	D
ATOM	4084	NZ	LYS D 140					
MOTA	4085	C	LYS D 140	90.660	39.339	9.068	1.00 19.16	D
MOTA	4086	0	LYS D 140	91.091	38.217	9.312	1.00 19.77	D
MOTA	4087	N	SER D 141	89.670	39.552	8.207	1.00 21.60	Ð
MOTA	4088	CA	SER D 141	89.030	38.438	7.507	1.00 23.19	D
		СВ	SER D 141	87.859	38.948	6.653	1.00 24.88	D
MOTA	4089					5.655	1.00 28.69	D
MOTA	4090	OG	SER D 141	88.288	39.858			
ATOM	4091	С	SER D 141	89.989	37.605	6.636	1.00 23.26	D
ATOM	4092	0	SER D 141	89.692	36.454	6.327	1.00 23.33	D
MOTA	4093	N	ASP D 142	91.137	38.159	6.251	1.00 21.38	D
ATOM	4094	CA	ASP D 142	92.075	37.387	5.429	1.00 22.54	D
ATOM	4095	СВ	ASP D 142	92.834	38.303	4.466	1.00 25.84	D
				93.943	39.064	5.143	1.00 29.78	D
ATOM	4096	CG	ASP D 142					D
MOTA	4097		ASP D 142	93.760	39.486	6.309	1.00 31.16	
ATOM	4098	OD2	ASP D 142	94.997	39.246	4.500	1.00 34.64	D
MOTA	4099	С	ASP D 142	93.045	36.637	6.336	1.00 22.89	D
MOTA	4100	0	ASP D 142	94.027	36.037	5.883	1.00 20.54	D
ATOM	4101	N	HIS D 143	92.753	36.700	7.632	1.00 21.06	D
					36.020	8.659	1.00 19.58	D
MOTA.	4102	CA	HIS D 143	93.522				Ď
MOTA	4103	CB	HIS D 143	93.628	34.534	8.317	1.00 19.03	
ATOM	4104	CG	HIS D 143	92.295	33.892	8.104	1.00 23.00	D
MOTA	4105	CD2	HIS D 143	91.827	33.108	7.104	1.00 24.78	D
ATOM	4106	ND1	HIS D 143	91.237	34.087	8.967	1.00 21.97	D
ATOM	4107		HIS D 143	90.174	33.455	8.505	1.00 24.67	Ð
			HIS D 143	90.504	32.853	7.375	1.00 24.72	D
MOTA	4108						1.00 20.11	D
MOTA	4109	C	HIS D 143	94.878	36.602	8.986		
MOTA	4110	0	HIS D 143	95.691	35.962	9.654	1.00 21.09	D
MOTA	4111	N	SER D 144	95.118	37.820	8.514	1.00 21.24	D
MOTA	4112	CA	SER D 144	96.352	38.525	8.826	1.00 21.79	D
ATOM	4113	СВ	SER D 144	96.834	39.353	7.627	1.00 20.33	D
		OG	SER D 144	96.047	40.511	7.434	1.00 24.32	D
MOTA	4114				39.440	9.990	1.00 21.43	D
ATOM	4115	C	SER D 144	95.940				D
ATOM	4116	0	SER D 144	94.830	39.317	10.504	1.00 20.74	
ATOM	4117	N	PHE D 145	96.809	40.352	10.412	1.00 21.56	D
ATOM	4118	CA	PHE D 145	96.463	41.235	11.523	1.00 22.54	D
MOTA	4119	CB	PHE D 145	97.156	40.791	12.817	1.00 22.63	D
ATOM	4120	CG	PHE D 145	96.896	39.368	13.200	1.00 25.73	D
			1 PHE D 145	97.565	38.329	12.562	1.00 26.67	D
MOTA	4121				39.063	14.207	1.00 23.65	D
ATOM	4122		2 PHE D 145	95.987			1.00 27.30	D
MOTA	4123		1 PHE D 145	97.333	37.004	12.921		
ATOM	4124	CE:	2 PHE D 145	95.750	37.746	14.572	1.00 25.43	D
ATOM	4125	CZ	PHE D 145	96.426	36.713	13.926	1.00 24.90	D
ATOM	4126	C	PHE D 145	96.850	42.687	11.299	1.00 22.51	D
ATOM	4127	ō	PHE D 145	97.540		10.339	1.00 23.97	D
			PHE D 146	96.371	43.540	12.198	1.00 20.96	D
MOTA	4128	N.		96.729	44.946	12.190	1.00 19.68	D
MOTA	4129	CA					1.00 17.70	D
ATOM	4130			95.696		11.439		
MOTA	4131					12.159	1.00 15.76	D
MOTA	4132	CD	1 PHE D 146	94.201	47.173	12.948	1.00 16.08	D
ATOM	4133		2 PHE D 146		45.170	11.976	1.00 14.70	D
ATOM	4134		1 PHE D 146	92.961		13.543	1.00 13.47	D
			2 PHE D 146			12.563	1.00 15.43	D
MOTA	4135						1.00 14.68	D
MOTA	4136							D
MOTA	4137		PHE D 146					
MOTA	4138	0	PHE D 146					D
MOTA	4139	N	LYS D 147	97.666	46.379	13.901	1.00 20.23	D

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MOTA	4140	CA	LYS D 14		46.817	15.260	1.00 19.84	D
MOTA	4141	CB	LYS D 14	7 99.184	46.148	15.796	1.00 21.50	D
ATOM	4142	CG	LYS D 14	7 99.651	46.679	17.134	1.00 24.87	D
MOTA	4143	CD	LYS D 14	7 100.764	45.832	17.724	1.00 27.18	D
ATOM	4144	CE	LYS D 14		44.515	18.253	1.00 31.41	D
					43.984	19.341	1.00 32.97	D
ATOM	4145	NZ	LYS D 14					
MOTA	4146	С	LYS D 14		48.324	15.274	1.00 18.69	D
ATOM	4147	0	LYS D 14	7 98.603	48.914	14.352	1.00 20.14	D
ATOM	4148	N	ILE D 14	8 97.497	48.944	16.314	1.00 18.22	D
ATOM	4149	CA	ILE D 14		50.387	16.446	1.00 18.25	D
			ILE D 14		50.942	16.548	1.00 20.80	D
ATOM	4150	CB						
ATOM	4151	CG2			52.459	16.659	1.00 22.44	D
MOTA	4152	CG1	ILE D 14	18 95.308	50.533	15.292	1.00 23.89	D
MOTA	4153	CD1	ILE D 14	18 93.840	50.858	15.314	1.00 24.42	D
ATOM	4154	C	ILE D 14	18 98.369	50.816	17.646	1.00 19.71	D
MOTA	4155	0	ILE D 14		50.294	18.757	1.00 17.77	D
ATOM	4156	N	SER D 14		51.753	17.395	1.00 19.08	D
							1.00 18.19	D
MOTA	4157	CA	SER D 14		52.278	18.424		
MOTA	4158	CB	SER D 14	19 101.633	52.137	17.991	1.00 18.51	D
MOTA	4159	OG	SER D 14	19 102.518	52.492	19.040	1.00 19.49	D
ATOM	4160	C	SER D 14	99.839	53.744	18.646	1.00 18.14	D
ATOM	4161	0	SER D 14		54.490	17.693	1.00 18.17	D
			TYR D 1		54.155	19.905	1.00 16.95	D
ATOM	4162	N						D
MOTA	4163	CA	TYR D 19		55.524	20.261	1.00 16.12	
MOTA	4164	CB	TYR D 1	50 98.310	55.524	21.213	1.00 15.57	D
MOTA	4165	CG	TYR D 15	50 97.116	54.750	20.701	1.00 16.81	D
ATOM	4166	CD1	TYR D 1	50 96.291	55.276	19.709	1.00 14.33	D
ATOM	4167		TYR D 1		54.554	19.222	1.00 17.50	D
ATOM	4168		TYR D 1		53.486	21.199	1.00 15.90	D
						20.719	1.00 18.41	D
ATOM	4169				52.760			
ATOM	4170	CZ	TYR D 1		53.297	19.732	1.00 16.27	D
ATOM	4171	OH	TYR D 1	50 93.868	52.574	19.244	1.00 20.03	D
ATOM	4172	С	TYR D 1	50 100.650	56.266	20.922	1.00 16.35	D
MOTA	4173	0	TYR D 1	50 101.438	55.690	21.669	1.00 16.95	D
ATOM	4174	N	LEU D 1		57.558	20.643	1.00 16.64	D
						21.227	1.00 16.50	ם
ATOM	4175	CA	LEU D 1		58.396			
MOTA	4176	CB	LEU D 1		58.705	20.203	1.00 15.48	D
MOTA	4177	CG	LEU D 1	51 103.806	59.825	20.639	1.00 17.55	D
MOTA	4178	CD1	LEU D 1	51 104.641	59.374	21.834	1.00 16.60	D
MOTA	4179	CD2	LEU D 1	51 104.702	60.213	19.476	1.00 16.11	D
ATOM	4180	C	LEU D 1			21.693	1.00 17.56	D
						20.888	1.00 17.18	D
MOTA	4181	0	LEU D 1				1.00 16.14	D
MOTA	4182	N	THR D 1			22.983		
ATOM	4183	CA	THR D 1	Ş2 100.690		23.448	1.00 19.47	D
MOTA	4184	CB	THR D 1	52 100.359	61.248	24.966	1.00 21.24	D
MOTA	4185	OG1	THR D 1	52 101.517	60.871	25.725	1.00 25.03	Ø
MOTA	4186	CG2	THR D 1	52 99.214	60.281	25.247	1.00 20.79	D
ATOM	4187	C	THR D 1			23.151	1.00 19.82	D
						23.218	1.00 21.31	Ð
MOTA	4188	0	THR D 1					D
MOTA	4189	N	LEU D 1			22.781	1.00 20.76	
MOTA	4190	CA	LEU D 1			22.488	1.00 24.15	D
MOTA	4191	CB	LEU D 1			21.089	1.00 25.45	D
MOTA	4192	CG	LEU D 1	53 101.959	64.575	19.785	1.00 27.17	D
ATOM	4193		LEU D 1			19.986	1.00 27.83	D
MOTA	4194		LEU D 1			19.319	1.00 27.38	D
						22.601	1.00 25.73	D
MOTA	4195	С	LEU D 1					
MOTA	4196	0	LEU D 1			22.681	1.00 26.55	D
ATOM	4197	N	LEU D 1			22.640	1.00 26.77	D
MOTA	4198	CA	LEU D 1	.54 101.781	. 68.369	22.734	1.00 26.34	D
MOTA	4199	CB	LEU D 1	.54 102.298	69.027	24.019	1.00 25.08	D
ATOM	4200	CG	LEU D 1			24.288	1.00 26.28	D
			LEU D 1			24.570	1.00 24.44	D
ATOM	4201						1.00 23.08	D
ATOM	4202		LEU D 1			25.477		
ATOM	4203	C	TEA D 1			21.522	1.00 28.41	D
ATOM	4204	0	LEU D 1	.54 103.577	7 69.327	21.468	1.00 27.19	D
MOTA	4205	N	PRO D 1	.55 101.534	69.351	20.523	1.00 30.32	Œ
MOTA	4206	CD	PRO D 1			20.453	1.00 30.25	D
ATOM	4207	CA	PRO D 1			19.294	1.00 31.71	D
			PRO D				1.00 31.92	D
MOTA	4208	CB					1.00 31.51	D
ATOM	4209	CG	PRO D			18.963		
MOTA	4210	C	PRO D 1			19.508	1.00 35.12	D
MOTA	4211	0	PRO D			20.112	1.00 35.64	D
MOTA	4212	N	SER D	L56 103.89	3 71.436	19.014	1.00 39.00	D
ATOM	4213	CA	SER D	104.70	72.643	19.083	1.00 42.94	D

MOTA	4214	CB	SER D	156	105.819	72.492	20.121	1.00 43.03	D
MOTA	4215	OG	SER D	156	105.288	72.385	21.430	1.00 45.30	D
ATOM	4216	C	SER D	156	105.311	72.763	17.694	1.00 46.03	D
MOTA	4217	ō	SER D		104.875	72.084	16.770	1.00 47.06	D
ATOM		N	ALA D		106.316	73.609	17.534	1.00 49.61	D
	4218								
MOTA	4219	CA	ALA D		106.931	73.756	16.222	1.00 51.03	D
MOTA	4220	CB	ALA D		106.977	75.231	15.828	1.00 51.20	D
ATOM	4221	C	ALA D	157	108.334	73.163	16.195	1.00 51.50	D
ATOM	4222	0	ALA D	157	108.985	73.147	15.150	1.00 52.20	D
ATOM	4223	N	GLU D	158	108.797	72.669	17.339	1.00 52.37	D
ATOM	4224	CA	GLU D		110.141	72.103	17.411	1.00 53.43	D
ATOM	4225	СВ	GLU D		110.946	72.785	18.524	1.00 57.17	D
									Ď
ATOM	4226	CG	GLU D		110.401	72.570	19.934	1.00 61.50	
ATOM	4227	CD	GLA D		109.278	73.529	20.291	1.00 63.75	D
MOTA	4228	OE1	GTO D	158	108.757	73.431	21.425	1.00 63.56	D
MOTA	4229	OB2	GLU D	158	108.922	74.381	19.445	1.00 65.17	D
ATOM	4230	C	GLU D	158	110.190	70.592	17.614	1.00 51.03	D
ATOM	4231	0	GLU D	158	111.103	70.084	18.265	1.00 51.07	D
ATOM	4232	N	GLU D		109.219	69.876	17.057	1.00 47.47	D
			GLU D		109.185	68.425	17.193	1.00 46.22	D
ATOM	4233	CA							ם
ATOM	4234	СВ	GLA D		108.337	68.013	18.406	1.00 47.11	
ATOM	4235	CG	GLU D		109.127	67.692	19.671	1.00 48.53	D
ATOM	4236	æ	GLU D	159	108.268	67.042	20.751	1.00 50.37	D
MOTA	4237	OE1	GLU D	159	107.319	67.694	21.238	1.00 50.39	D
ATOM	4238	OE2	GLU D	159	108.537	65.873	21.112	1.00 50.03	D
ATOM	4239	C	GLU D		108.641	67.714	15.960	1.00 43.84	D
ATOM	4240	ō	GLU D		107.515	67.974	15.535	1.00 44.12	D
ATOM		N	SER D		109.443	66.825	15.380	1.00 39.56	D
	4241						14.229		D
MOTA	4242	CA	SER D		108.993	66.054		1.00 37.29	
ATOM	4243	CB	SER D		109.971	66.172	13.055	1.00 37.41	D
ATOM	4244	OG	SER D	160	111.070	65.298	13.206	1.00 41.72	D
MOTA	4245	C	SER D	160	108.933	64.615	14.734	1.00 35.08	D
ATOM	4246	0	SER D	160	109.754	64.207	15.557	1.00 33.66	D
ATOM	4247	N	TYR D		107.961	63.846	14.260	1.00 32.11	D
ATOM	4248	CA	TYR D		107.828	62.478	14.728	1.00 29.69	D
								1.00 29.62	D
ATOM	4249	CB	TYR D		106.550	62.315	15.547		
MOTA	4250	CG	TYR D		106.347	63.349	16.620	1.00 29.33	D
ATOM	4251	CD1	TYR D	161	105.761	64.577	16.327	1.00 31.31	D
MOTA	4252	CE1	TYR D	161	105.513	65.515	17.329	1.00 32.70	D
ATOM	4253	CD2	TYR D	161	106.695	63.085	17.937	1.00 30.13	D
ATOM	4254	CE2	TYR D	161	106.457	64.013	18.947	1.00 30.43	ם
ATOM	4255	CZ	TYR D		105.863	65.223	18.638	1.00 31.92	D
ATOM	4256	OH	TYR D		105.592	66.128	19.643	1.00 35.12	D
						61.441	13.627	1.00 29.60	D
MOTA	4257	C	TYR D		107.820				
MOTA	4258	0	TYR D		107.493	61.728	12.473	1.00 29.45	D
ATOM	4259	N	ASP D		108.172	60.221	14.005	1.00 29.35	ם
ATOM	4260	CA	ASP D	162	108.201	59.109	13.075	1.00 30.15	D
ATOM	4261	CB	ASP D	162	109.618	58.863	12.548	1.00 34.90	D
MOTA	4262	CG	ASP D	162	110.154	60.016	11.733	1.00 37.70	D
MOTA	4263		ASP D	162	109.669	60.218	10.597	1.00 40.13	D
ATOM	4264		ASP D		111.061	60.716	12.235	1.00 38.68	D
		C	ASP D		107.759	57.851	13.784	1.00 29.84	D
MOTA	4265	-						1.00 26.72	D
MOTA	4266	0	ASP D		108.010	57.672	14.978		
MOTA	4267	N	CYS I		107.088	56.984	13.039	1.00 29.31	D
MOTA	4268	CA	CYS I		106.684	55.700	13.569	1.00 29.59	D
ATOM	4269	C	CYS I	163	107.689	54.769	12.902	1.00 28.04	D
MOTA	4270	0	CYS I	163	107.822	54.772	11.685	1.00 26.22	D
MOTA	4271	CB	CYS I	163	105.265	55.326	13,134	1.00 29.11	D
ATOM	4272	SG	CYS I		104.703	53.760	13.878	1.00 34.32	D
	4273	N	LYS I		108.417	54.001	13.699	1.00 29.03	D
ATOM			LYS I				13.161	1.00 29.67	D
ATOM	4274	CA			109.404	53.072			
MOTA	4275	CB	LYS I		110.730	53.238	13.911	1.00 32.54	D
MOTA	4276	CG	LYS I		111.874	52.352	13.416	1.00 34.76	D
MOTA	4277	CD	LYS I		113.109	52.528	14.297	1.00 34.79	D
ATOM	4278	CE	LYS I	164	114.254	51.630	13.850	1.00 38.29	D
MOTA	4279	NZ	LYS I		115.425	51.702	14.775	1.00 36.58	D
ATOM	4280	C	LYS I		108.863	51.651	13.322	1.00 28.94	D
ATOM	4281	Ö	LYS I		108.642	51.189	14.443	1.00 29.32	D
			VAL			50.974	12.197	1.00 27.33	ם
MOTA	4282	N			108.632				
MOTA	4283	CA	VAL		108.100	49.618	12.212	1.00 26.58	D
MOTA	4284	СВ	VAL I		106.797	49.516	11.359	1.00 27.12	D
ATOM	4285		VAL I		106.199	48.122	11.462	1.00 25.56	D
MOTA	4286	CG	VAL I		105.787	50.544	11.827	1.00 27.97	D
ATOM	4287	С	VAL I	165	109.113	48.600	11.690	1.00 26.91	D

MOTA	4288	0	VAL D	165	109.621	48.720	10.583	1.00 25.56	D
ATOM	4289	N	GLU D	166	109.414	47.606	12.513	1.00 28.75	D
ATOM	4290	CA	GLU D	166	110.338	46.544	12.139	1.00 30.67	D
ATOM	4291	CB	GLU D		111.445	46.410	13.194	1.00 33.57	ם
		CG	GLU D		112.452	47.565	13.142	1.00 41.68	D
MOTA	4292								D
ATOM	4293	CD	GLU D		113.506	47.526	14.244	1.00 46.12	
MOTA	4294		GLU D		114.482	48.304	14.146	1.00 49.01	D
MOTA	4295	OE2	GLU D	166	113.363	46.736	15.206	1.00 49.40	D
MOTA	4296	C	GLU D	166	109.543	45.243	12.008	1.00 30.18	D
ATOM	4297	0	GLU D	166	108.737	44.900	12.878	1.00 28.51	D
ATOM	4298	N	HIS D		109.759	44.535	10.907	1.00 29.48	D
ATOM	4299	CA	HIS D		109.056	43.281	10.648	1.00 30.29	D
					107.686		10.025	1.00 29.56	D
ATOM	4300	CB	HIS D			43.569			
ATOM	4301	CG	HIS D		106.808	42.363	9.903	1.00 30.02	D
MOTA	4302	CD2	HIS D	167	106.562	41.541	8.856	1.00 29.91	D
MOTA	4303	ND1	HIS D	167	106.068	41.871	10.957	1.00 31.27	D
MOTA	4304	CE1	HIS D	167	105.404	40.798	10.564	1.00 28.43	D
MOTA	4305	NE2	HIS D	167	105.687	40.576	9.293	1.00 28.97	D
ATOM	4306	C	HIS D		109.886	42.440	9.684	1.00 30.36	D
		ō	HIS D		110.607	42.976	8.842	1.00 30.66	D
ATOM	4307						9.801	1.00 31.13	D
MOTA	4308	N	TRP D		109.775	41.122			Ď
MOTA	4309	CA	TRP D		110.521	40.219	8.930	1.00 32.08	
MOTA	4310	CB	TRP D	168	110.270	38.765	9.336	1.00 28.28	a
ATOM	4311	CG	TŘP D	168	110.665	38.475	10.739	1.00 26.36	D
MOTA	4312	CD2	TRP D	168	110.031	37.556	11.635	1.00 25.51	D
ATOM	4313	CE2		168	110.759	37.578	12.842	1.00 26.35	D
ATOM	4314	CE3			108.916	36.715	11.534	1.00 24.88	D
			TRP D		111.721	39.004	11.416	1.00 27.27	D
MOTA	4315						12.682	1.00 28.25	D
ATOM	4316		TRP D		111.786	38.471			
ATOM	4317	CZ2			110.412	36.791	13.943	1.00 27.00	D
MOTA	4318	CZ3	TRP D	168	108.568	35.932	12.628	1.00 25.90	D
MOTA	4319	CH2	TRP D	168	109.315	35.976	13.817	1.00 26.65	D
ATOM	4320	С	TRP D	168	110.180	40.403	7.452	1.00 33.22	D
ATOM	4321	0	TRP D	168	111.011	40.139	6.582	1.00 33.90	מ
ATOM	4322	N	GLY D		108.959	40.853	7.174	1.00 34.75	D
		CA	GLY D		108.533	41.060	5.797	1.00 36.14	D
MOTA	4323						5.215	1.00 37.80	D
MOTA	4324	C	GLY D		109.056	42.359			
MOTA	4325	0	GLY D		108.635	42.796	4.139	1.00 36.95	D
MOTA	4326	N	TEO D	170	109.979	42.981	5.938	1.00 38.89	D
ATOM	4327	CA	TEO D	170	110.578	44.234	5.509	1.00 40.79	D
ATOM	4328	CB	LEU D	170	110.212	45.356	6.480	1.00 39.77	D
MOTA	4329	CG	TEO D		108.745	45.765	6.581	1.00 39.57	D
ATOM	4330		LEU D		108.592	46.809	7.671	1.00 38.10	D
	4331		LEUD		108.267	46.308	5.243	1.00 39.58	D
ATOM					112.092	44.085	5.465	1.00 42.12	D
MOTA	4332	C	LEU D						D
	4333	0	LEU D		112.688	43.506	6.370	1.00 41.54	
ATOM	4334	N	ASP D	171	112.706	44.613	4.411	1.00 45.36	D
MOTA	4335	CA	ASP D	171	114.158	44.559	4.252	1.00 48.35	D
MOTA	4336	CB	ASP D	171	114.539	44.947	2.820	1.00 50.69	D
MOTA	4337	CG	ASP D	171	113.467	45.775	2.137	1.00 52.75	D
ATOM	4338	ODI	L ASP D		113.076	46.827	2.689	1.00 54.19	D
ATOM	4339		ASP D		113.012	45.372	1.046	1.00 54.32	D
		c	ASP D		114.849	45.485	5.255	1.00 48.43	D
MOTA	4340					45.090	5.910	1.00 48.29	D
MOTA	4341	0	ASP D		115.816				
ATOM	4342	N	LYS D		114.348	46.715	5.364	1.00 48.92	D
MOTA	4343	CA	LYS D		114.883	47.707	6.299	1.00 49.86	D
MOTA	4344	CB	LYS D	172	115.502	48.898	5.552	1.00 51.58	Ð
MOTA	4345	CG	LYS D	172	116.667	48.566	4.637	1.00 55.86	D
MOTA	4346	CD	LYS D		116.203	47.963	3.316	1.00 58.23	D
ATOM	4347	CE	LYS D		115.408	48.966	2.493	1.00 59.62	D
	4348	NZ	LYS D		114.946	48.368	1.211	1.00 59.53	D
MOTA						48.224	7.165	1.00 48.46	D
MOTA	4349	C	LYS D		113.734			1.00 48.43	D
MOTA	4350	0	LYS D		112.564	48.026	6.833		
MOTA	4351	N	PRO D		114.050	48.885	8.291	1.00 46.54	D
ATOM	4352	æ	PRO D	173	115.355	49.048	8.954	1.00 46.03	D
ATOM	4353	CA	PRO D	173	112.974	49.400	9.137	1.00 44.41	D
ATOM	4354	СВ			113.722	50.029		1.00 44.19	D
ATOM	4355				114.950	49.197			D
			PRO D		112.180				D
MOTA	4356								D
ATOM	4357		PRO I		112.746				
MOTA	4358		TEO I		110.869				D
MOTA	4359				110.023	_			D
MOTA	4360	CB	LEO I	174	108.675				D
MOTA	4361	ÇG	LEU I	174	107.900	51.223	6.303	1.00 40.55	D

MOTA	4362	CD1	TEA I	174	106.637	50.397	6.151	1.00 42.25	ם
ATOM	4363		LEU I		107.568	52.698	6.448	1.00 42.67	D
MOTA	4364	C	LEU I		109.845	52.586	8.753	1.00 39.80	D
MOTA	4365	0	TEG I		109.645	52.420 53.792	9.955 8.200	1.00 39.99 1.00 38.49	D D
MOTA MOTA	4366 4367	n Ca	TEO I		109.947 109.787	55.016	8.983	1.00 38.04	ם
ATOM	4368	CB	TEO I		111.095	55.812	9.045	1.00 38.62	D
ATOM	4369	CG	TEO I		112.127	55.442	10.113	1.00 38.70	D
MOTA	4370	CD1	LEU I	175	111.518	55.648	11.489	1.00 39.24	D
MOTA	4371	CD2	LEU I	175	112.577	54.001	9.936	1.00 40.07	D
ATOM	4372	C	TEO 1		108.712	55.892	8.372	1.00 37.31	D
MOTA	4373	0		175	108.885	56.432	7.282	1.00 38.54	D
ATOM	4374	N		176	107.599	56.033 56.850	9.076	1.00 35.14	D D
ATOM	4375	CA CB	LYS I	D 176	106.511 105.175	56.124	8.577 8.768	1.00 33.88	D
ATOM ATOM	4376 4377	CG		D 176	104.204	56.325	7.620	1.00 36.72	Ď
ATOM	4378	CD		176	104.829	55.887	6.295	1.00 37.68	D
ATOM	4379	CE		176	103.820	55.913	5.155	1.00 39.32	D
ATOM	4380	NZ	LYS I	176	103.195	57.254	4.974	1.00 40.75	D
MOTA	4381	C		176	106.523	58.166	9.335	1.00 32.22	D
MOTA	4382	0		176	106.272	58.204	10.537	1.00 32.35	D
MOTA	4383	N		D 177 D 177	106.825 106.897	59.243 60.563	8.625 9.229	1.00 29.85 1.00 29.87	D D
MOTA MOTA	4384 4385	CA CB		D 177	107.836	61.456	8.411	1.00 30.84	ā
ATOM	4386	CG		D 177	108.014	62.830	8.979	1.00 31.41	Ď
MOTA	4387		HIS I		107.607	64.042	8.529	1.00 32.01	D
MOTA	4388	ND1	HIS I	D 177	108.695	63.067	10.155	1.00 32.16	D
ATOM	4389		HIS !		108.704	64.365	10.402	1.00 30.49	D
ATOM	4390		HIS		108.051	64.979	9.431	1.00 31.08	D
ATOM	4391	C		D 177	105.532	61.228	9.332	1.00 29.28 1.00 27.97	D D
MOTA	4392	o N		D 177 D 178	104.709 105.295	61.121 61.922	8.429 10.439	1.00 27.37	D
MOTA MOTA	4393 4394	CA	TRP		104.031	62.617	10.619	1.00 29.38	D
ATOM	4395	CB		D 178	103.518	62.464	12.048	1.00 26.73	D
ATOM	4396	CG		D 178	102.205	63.165	12.243	1.00 27.32	D
ATOM	4397	CD2	TRP	D 178	101.939	64.262	13.122	1.00 24.87	D
ATOM	4398	CE2	TRP		100.580	64.608	12.959	1.00 26.97	D
ATOM	4399	CE3		D 178	102.714	64.986	14.033	1.00 26.15	D
MOTA	4400		TRP		101.028	62.898 63.759	11.599 12.023	1.00 26.41 1.00 25.31	D D
MOTA	4401 4402		TRP TRP		100.050 99.980	65.649	13.675	1.00 25.60	D
ATOM ATOM	4403	CZ3		D 178	102.118	66.021	14.746	1.00 27.98	D
ATOM	4404			D 178	100.763	66.340	14.562	1.00 27.02	D
MOTA	4405	C		D 178	104.185	64.100	10.294	1.00 30.33	D
ATOM	4406	0		D 178	104.756	64.824	11,143	1.00 29.85	D
ATOM	4407	OXT		D 178	103.745	64.512	9.193	1.00 32.23	D
ATOM	4408	СВ	SER		113.641	35.776	8.019 8.608	1.00 59.19 1.00 59.65	E
ATOM	4409 4410	C	SER SER		112.349 114.352	35.748 33.977	9.601	1.00 57.92	E
MOTA MOTA	4411	0	SER		114.571	32.945	8.970	1.00 57.45	E
ATOM	4412	N	SER		116.055	35.305	8.352	1.00 59.31	E
MOTA	4413	CA	SER	E 3	114.719	35.342	9.020	1.00 58.85	E
MOTA	4414	N	PRO		113.799	33.958	10.824	1.00 56.65	E
MOTA	4415	CD	PRO		113.679	35.092	11.759	1.00 56.20	E
ATOM	4416	CA	PRO		113.403 113.362	32.704 33.086	11.472 12.946	1.00 55.50 1.00 56.49	e
ATOM ATOM	4417 4418	CB CG	PRO PRO		112.870	34.493	12.893	1.00 56.56	E
MOTA	4419	C	PRO		112.046	32.217	10.957	1.00 53.68	B
ATOM	4420	ō	PRO		111.168	33.024	10.648	1.00 54.06	E
MOTA	4421	N	GLU	E 5	111.875	30.903	10.855	1.00 51.52	E
MOTA	4422	CA	GLU		110.610	30.360	10.373	1.00 49.69	E
MOTA	4423	СВ	GLU		110.831	29.007	9.676	1.00 53.42	e
MOTA	4424	CG	GLU		111.305	27.867 26.626	10.561 9.758	1.00 57.99 1.00 60.86	B
ATOM ATOM	4425 4426	CD OF 1	GLU GLU.		111.671 110.857	26.196	8.908	1.00 62.41	E
ATOM	4427		GLU		112.772	26.077	9.979	1.00 63.42	E
ATOM	4428	C	GLU		109.619	30.231	11.525	1.00 45.48	E
MOTA	4429	0	GLU		109.919	29.644	12.564	1.00 46.07	B
ATOM	4430	N	ASP		108.436	30.800	11.337	1.00 40.87	E
MOTA	4431	CA	ASP		107.403	30.782	12.363	1.00 36.20 1.00 35.53	e
MOTA	4432 4433	CB CG	ASP ASP		106.911 105.995	32.214 32.323	12.617 13.827	1.00 35.53	E
MOTA MOTA	4434		ASP L ASP		105.395	33.268	13.864	1.00 34.88	E
ATOM	4435		ASP		106.089	31.487		1.00 33.84	E

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ATOM	4436	C	ASP		6	106.229	29.915	11.938	1.00 33.07	B
MOTA	4437	0	ASP	B	6	105.882	29.867	10.762	1.00 32.95	B
ATOM	4438	N	PHR	B	7	105.632	29.228	12.906	1.00 31.08	E
ATOM	4439	CA	PHE	E	7	104.466	28.380	12.669	1.00 29.18	B
ATOM	4440	СВ		B	7	104.760	26.950	13.116	1.00 31.11	B
ATOM			PHE		7	105.833	26.278	12.305	1.00 31.97	E
	4441	CG								
MOTA	4442			E	7	105.544	25.745	11.053	1.00 31.67	E
ATOM	4443	CD2	PHE	В	7	107.141	26.200	12.782	1.00 32.49	E
ATOM	4444	CE1	PHE	E	7	106.546	25,141	10.282	1.00 33.41	E
ATOM	4445	CE2	PHE	B	7	108.148	25.602	12.023	1.00 32.29	B
MOTA	4446	cz		E	7	107.850	25.071	10.770	1.00 31.62	E
ATOM	4447	C		E	7	103.345	28.994	13.504	1.00 27.19	E
MOTA	4448	0	PHE		7	103.483	29.151	14.715	1.00 25.77	E
MOTA	4449	N	VAL	E	8	102.238	29.340	12.855	1.00 25.52	E
MOTA	4450	CA	VAL	E	8	101.127	29.998	13.538	1.00 23.97	E
MOTA	4451	CB	VAL	B	8	100.903	31.411	12.949	1.00 22.51	E
ATOM	4452	CG1			8	99.789	32.130	13.703	1.00 20.58	E
ATOM	4453	CG2	VAL		8	102.205	32.211	13.002	1.00 22.51	E
MOTA	4454	С	VAL	E	8	99.785	29.275	13.510	1.00 24.21	E
ATOM	4455	0	VAL	E	8	99.369	28.736	12.485	1.00 25.26	E
ATOM	4456	N	TYR	E	9	99.096	29.288	14.643	1.00 23.98	E
ATOM	4457	CA	TYR	B	9	97.786	28.663	14.724	1.00 23.53	E
MOTA	4458	CB	TYR		9	97.796	27.505	15.718	1.00 24.07	B
ATOM	4459	CG	TYR		9	96.562	26.640	15.627	1.00 25.27	E
ATOM	4460	CD1	TYR	E	9	96.570	25.460	14.889	1.00 27.68	E
ATOM	4461	CE1	TYR	E	9	95.435	24.658	14.801	1.00 27.67	E
ATOM	4462	CD2	TYR	E	9	95.384	27.002	16.272	1.00 24.82	E
ATOM	4463	CE2	TYR		9	94.245	26.211	16.191	1.00 25.29	E
		cz	TYR		9	94.277	25.040	15.458	1.00 26.82	B
ATOM	4464									
MOTA	4465	OH	TYR		9	93.163	24.240	15.403	1.00 27.65	B
MOTA	4466	C	TYR	B	9	96.775	29.707	15.179	1.00 23.14	E
MOTA	4467	0	TYR	E	9	97.037	30.476	16.106	1.00 23.66	E
ATOM	4468	N	GLN	E	10	95.622	29.739	14.523	1.00 21.64	E
MOTA	4469	CA	GLN		10	94.582	30.686	14.892	1.00 21.14	E
		CB	GLN		10	94.438	31.793	13.843	1.00 20.35	B
ATOM	4470									E
MOTA	4471	CG	GLN		10	95.677	32.598	13.529	1.00 19.58	
ATOM	4472	æ	GLN		10	95.410	33.655	12.461	1.00 18.44	B
ATOM	4473	OE1	GLN	E	10	94.498	34.474	12.593	1.00 19.00	器
MOTA	4474	NE2	GLN	E	10	96.206	33.640	11.400	1.00 18.89	E
MOTA	4475	С	GLN	E	10	93.232	29.997	15.006	1.00 19.74	E
ATOM	4476	ō	GLN		10	92.904	29.113	14.223	1.00 21.71	E
							30.408	15.991	1.00 19.13	E
ATOM	4477	N	PHE		11	92.450				
ATOM	4478	CA	PHE		11	91.108	29.887	16.145	1.00 16.86	E
ATOM	4479	CB	PHE	E	11	90.981	28.881	17.271	1.00 16.74	B
ATOM	4480	CG	PHE	E	11	89.562	28.466	17.517	1.00 18.71	E
MOTA	4481	CD1	PHE	В	11	88.910	27.615	16.626	1.00 21.10	E
ATOM.	4482	CD2	PHE	E	11	88.849	28.985	18.595	1.00 18.11	E
ATOM	4483		PHE		11	87.559	27.290	16.807	1.00 22.40	E
										E
ATOM	4484		PHE		11	87.499	28.671	18.789	1.00 15.75	
ATOM	4485	CZ	PHE		11	86.854	27.826	17.898	1.00 21.25	E
MOTA	4486	C	PHB	E	11	90.218	31.069	16.451	1.00 17.10	E
MOTA	4487	0	PHE	E	11	90.461	31.819	17.406	1.00 13.97	E
MOTA	4488	N	LYS	B	12	89.197	31.241	15.622	1.00 16.07	E
ATOM	4489	CA	LYS		12	88.266	32.338	15.789	1.00 16.96	E
ATOM	4490	CB	LYS		12	88.308	33.246	14.564	1.00 17.05	B
										B
MOTA	4491	CG	LYS		12	89.703	33.748	14.200	1.00 17.57	
MOTA	4492	æ	LYS		12	89.663	34.535	12.888	1.00 18.92	E
MOTA	4493	CE	LYS	E	12	91.018	35.136	12.532	1.00 17.07	B
MOTA	4494	NZ	LYS	E	12	90.920	36.063	11.362	1.00 14.26	E
ATOM	4495	С	LYS	E	12	86.856	31.803	15.987	1.00 17.87	. В
ATOM	4496	0	LYS		12	86.354	31.039	15.165	1.00 16.82	B
MOTA	4497	N	GLY		13	86.235	32.195	17.098	1.00 18.19	E
MOTA	4498	CA	GLY		13	84.875	31.776	17.391	1.00 19.62	8
ATOM	4499	С	GLY		13	83.991	32.939	17.010	1.00 19.93	E
ATOM	4500	0	GLY	E	13	83.539	33.695	17.868	1.00 21.65	E
ATOM	4501	N	MET	E	14	83.728	33.070	15.715	1.00 19.89	B
ATOM	4502	CA	MET		14	82.947	34.184	15.197	1.00 20.54	E
ATOM	4503	СВ	MET		14	83.430	34.490	13.785	1.00 21.02	E
ATOM	4504		MET		14	84.937	34.657	13.751	1.00 23.04	E
		CG								
MOTA	4505	SD	MET		14	85.587	35.218	12.190	1.00 25.32	E
ATOM	4506	CB	MET		14	85.218	36.938	12.284	1.00 20.32	E
ATOM	4507	C	MET	E	14	81,429	34.078	15.219	1.00 20.83	В
MOTA	4508	0	MET	E	14	80.859	32.999	15.101	1.00 20.77	E
MOTA	4509	N	CYS		15	80.789	35.232	15.377	1.00 20.66	E

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MOTA	4510	CA	CYS		15	79.332	35.336	15.418	1.00 22.09	B
ATOM	4511	C	CYS	E	15	78.882	36.495	14.524	1.00 21.39	B
MOTA	4512	0	CYS	B	15	79.393	37.614	14.644	1.00 19.38	E
ATOM	4513	СВ	CYS	ĸ	15	78.841	35.616	16.848	1.00 22.10	В
		SG	CYS		15	78.970	34.281	18.094	1.00 26.75	B
ATOM	4514									
MOTA	4515	N	TYR	E	16	77.931	36.229	13.633	1.00 20.94	B
ATOM	4516	CA	TYR	B	16	77.408	37.270	12.752	1.00 21.23	B
MOTA	4517	CB	TYR	R	16	77.548	36.858	11.287	1.00 18.37	B
						78.972	36.574	10.876	1.00 19.23	E
MOTA	4518	CG	TYR		16					
MOTA	4519	CD1	TYR	E	16	79.576	35.354	11.178	1.00 18.71	E
ATOM	4520	CE1	TYR	E	16	80.875	35.084	10.789	1.00 18.69	E
ATOM	4521		TYR		16	79.715	37.524	10.178	1.00 20.25	B
							37.270	9.785	1.00 17.18	E
ATOM	4522		TYR		16	81.022				
ATOM	4523	CZ	TYR		16	81.595	36.047	10.088	1.00 21.03	E
MOTA	4524	OH	TYR	B	16	82.872	35.775	9.662	1.00 22.99	E
ATOM	4525	C	TYR	E	16	75.938	37.543	13.085	1.00 22.17	E
		ō	TYR		16	75.132	36.612	13.199	1.00 21.71	B
ATOM	4526									
ATOM	4527	N	PHE		17	75.607	38.825	13.247	1.00 23.05	E
ATOM	4528	CA	PHE	E	17	74.254	39.263	13.591	1.00 23.67	E
ATOM	4529	CB	PHE	B	17	74.261	39.988	14.942	1.00 22.49	E
	4530	CG	PHE		17	74.813	39.172	16.084	1.00 25.10	B
ATOM										
MOTA	4531		PHE		17	74.007	38.270	16.772	1.00 24.22	E
ATOM	4532	CD2	PHE	E	17	76.140	39.318	16.482	1.00 24.67	E
ATOM	4533	CE1	PHE	E	17	74.516	37.526	17.844	1.00 24.68	E
			PHE		17	76.656	38.579	17.548	1.00 24.45	E
MOTA	4534									13
MOTA	4535	CZ	PHE	E	17	75.843	37.684	18.228	1.00 24.13	
MOTA	4536	C	PHE	E	17	73.673	40.223	12.549	1.00 25.10	E
ATOM	4537	0	PHE	В	17	74.390	41.034	11.971	1.00 24.65	E
		N	THR		18	72.365	40.122	12.333	1.00 27.15	E
ATOM	4538									B
MOTA	4539	CA	THR		18	71.638	40.983	11.405	1.00 29.69	
MOTA	4540	CB	THR	B	18	71.609	40.397	9.978	1.00 29.46	B
MOTA	4541	OG1	THR	E	18	72.949	40.252	9.500	1.00 32.31	E
MOTA	4542		THR		18	70.863	41.321	9.032	1.00 28.09	E
							41.080	11.950	1.00 31.56	E
MOTA	4543	С	THR		18	70.217				
ATOM	4544	0	THR	B	18	69.638	40.071	12.355	1.00 32.09	E
MOTA	4545	N	ASN	E	19	69.661	42.290	11.969	1.00 33.38	E
ATOM	4546	CA	ASN	12	19	68.316	42.495	12.497	1.00 35.02	E
						67.279	41.755	11.647	1.00 37.99	E
ATOM	4547	CB	ASN		19					
ATOM	4548	CG	ASN	E	19	66.779	42.587	10.489	1.00 42.21	E
MOTA	4549	OD1	ASN	E	19	66.271	43.695	10.687	1.00 47.70	E
ATOM	4550	ND2	ASN	E	19	66.910	42.063	9.273	1.00 43.13	E
			ASN		19	68.264	41.977	13.924	1.00 34.10	E
ATOM	4551	C								E
MOTA	4552	0	asn	E	19	67.487	41.077	14.233	1.00 34.27	
MOTA	4553	N	GLY	E	20	69.088	42.553	14.795	1.00 33.50	B
MOTA	4554	CA	GLY	R	20	69.120	42.106	16.175	1.00 33.61	E
		c	GLY		20	69.575	40.663	16.175	1.00 33.98	E
ATOM	4555,									B
ATOM	4556	0	GLY	R	20	70.580	40.343	15.541	1.00 34.56	
MOTA	4557	N	THR	E	21	68.847	39.789	16.866	1.00 34.08	B
ATOM	4558	CA	THR	E	21	69.198	38.372	16.897	1.00 35.71	E
ATOM	4559	CB	THR		21	69.193		18.335	1.00 37.69	E
							38.026	18.930	1.00 39.78	B
ATOM	4560		THR		21	67.907				E
MOTA	4561	CG2	THR	B	21	70.268	38.480	19.174	1.00 38.05	
MOTA	4562	С	THR	B	21	68.251	37.517	16.050	1.00 35.19	E
ATOM	4563	ō	THR		21	68.092	36.324	16.303	1.00 36.08	E
			GLU		22	67.619	38.129	15.052	1.00 34.15	B
ATOM	4564	N								E
MOTA	4565	CA	GLU		22	66.705	37.405	14.176	1.00 34.08	
MOTA	4566	CB	GLŪ	B	22	65.868	38.388	13.354	1.00 33.12	E
ATOM	4567	CG	GLU	E	22	64.781	39.073	14.164	1.00 33.66	E
ATOM	4568	CD	GLU		22	64.173	40.266	13.451	1.00 35.85	E
								12.244	1.00 35.10	E
MOTA	4569		. GLU		22	63.865	40.151			
MOTA	4570	OE2	GLU	E	22	63.995	41.317	14.105	1.00 38.34	E
ATOM	4571	C	GLU	E	22	67.523	36.503	13.265	1.00 33.80	E
MOTA	4572	ō	GLU		22	67.205	35.329	13.092	1.00 34.50	E
						68.574	37.065	12.678	1.00 33.59	E
ATOM	4573	N	ARG		23					
MOTA	4574	CA	ARG		23	69.467	36.298	11.818	1.00 33.75	E
ATOM	4575	CB	ARG	B	23	69.703	36.996	10.470	1.00 36.33	E
MOTA	4576	CG	ARG		23	68.599	36.815	9.434	1.00 42.06	E
			ARG		23	67.342	37.577	9.813	1.00 47.83	E
MOTA	4577	æ								B
MOTA	4578	NB	ARC		23	66.408	37.696	8.695	1.00 51.02	
ATOM	4579	CZ	ARC	3 E	23	65.349	38.502	8.690	1.00 52.66	B
MOTA	4580		L ARC		23	65.087	39.263	9.747	1.00 50.82	E
MOTA										_
	AFOR	PLEE .		ם ב	23	64 555	38 555	7.626	1.00 53.53	E
	4581	NH	2 ARC		23	64.555	38.555	7.626	1.00 53.53	
ATOM ATOM	4581 4582 4583	NH: C		3 E	23 23 23	64.555 70.788 71.465	38.555 36.177 37.172	7.626 12.560 12.827	1.00 53.53 1.00 30.98 1.00 30.90	e E

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MOTA	4584	N	VAL	B	24	71.149	34.955	12.909	1.00 28.33	B
MOTA	4585	CA	VAL	E	24	72.394	34.735	13.621	1.00 25.06	B
MOTA	4586	CB	VAL	E	24	72.148	34.500	15.129	1.00 22.98	B
ATOM	4587		VAL		24	73.456	34.106	15.817	1.00 21.05	E
		CG2			24	71.582	35.762	15.763	1.00 21.04	E
ATOM	4588								1.00 23.08	B
MOTA	4589	С	VAL		24	73.144	33.550	13.049		
MOTA	4590	0	VAL		24	72.600	32.458	12.914	1.00 24.17	E
ATOM	4591	N	ARG	E	25	74.398	33.778	12.694	1.00 23.02	E
MOTA	4592	CA	ARG	E	25	75.223	32.718	12.156	1.00 23.30	E
ATOM	4593	CB	ARG	E	25	75.511	32.930	10.659	1.00 24.06	E
ATOM	4594	CG	ARG		25	76.653	32.044	10.176	1.00 25.99	E
						76.470	31.478	8.774	1.00 28.29	E
ATOM	4595	CD	ARG		25				1.00 29.69	E
ATOM	4596	NB	ARG		25	76.468	32.502	7.743		
MOTA	4597	CZ	ARG	В	25	76.786	32.287	6.466	1.00 29.57	E
MOTA	4598	NH1	ARG	E	25	77.145	31.075	6.047	1.00 27.28	E
ATOM	4599	NH2	ARG	E	25	76.733	33.293	5.604	1.00 26.98	B
ATOM	4600	C	ARG	E	25	76.535	32.631	12.916	1.00 22.65	E
ATOM	4601	ŏ	ARG		25	77.261	33.620	13.041	1.00 22.47	E
						76.828	31.444	13.433	1.00 21.04	B
MOTA	4602	N	FEA		26					B
MOTA	4603	CA	LEU		26	78.069	31.227	14.152	1.00 21.94	
MOTA	4604	СВ	LEU	E	26	77.834	30.338	15.383	1.00 21.37	E
ATOM	4605	CG	LEU	E	26	79.054	29.778	16.128	1.00 22.89	E
ATOM	4606	CD1	LEU	E	26	78.723	29.567	17.602	1.00 25.16	E
ATOM	4607		LEU		26	79.483	28.466	15.493	1.00 23.51	B
		C	LEU		26	79.032	30.552	13.193	1.00 21.17	E
MOTA	4608						29.674	12.432	1.00 21.77	E
MOTA	4609	0	LEU		26	78.637				E
MOTA	4610	N	VAL		27	80.285	30.983	13.201	1.00 19.92	
ATOM	4611	CA	VAL	E	27	81.278	30.358	12.345	1.00 21.31	E
ATOM	4612	CB	VAL	E	27	81.530	31.166	11.039	1.00 20.44	E
MOTA	4613	CG1	VAL	В	27	82.524	30.420	10.156	1.00 21.63	B
ATOM	4614		VAL		27	80.221	31.366	10.275	1.00 20.48	E
	4615	C	VAL		27	82.581	30.231	13.112	1.00 21.74	B
ATOM						83.189	31.228	13.487	1.00 24.11	E
MOTA	4616	0	VAL		27				1.00 20.88	E
MOTA	4617	N	SER		28	82.994	29.001	13.383		
MOTA	4618	CA	SER	E	28	84.249	28.799	14.084	1.00 21.53	E
MOTA	4619	CB	SER	E	28	84.113	27.702	15.152	1.00 20.62	B
MOTA	4620	OG	SER	E	28	83.693	26.475	14.598	1.00 29.22	E
MOTA	4621	C	SER		28	85.274	28.433	13.006	1.00 21.41	E
	4622	ŏ	SER		28	84.992	27.631	12.105	1.00 19.11	E
MOTA						86.450	29.051	13.090	1.00 18.23	E
MOTA	4623	N	ARG		29				1.00 18.45	E
MOTA	4624	CA	ARG		29	87.496	28.838	12.105		
ATOM	4625	CB	ARG	B	29	87.701	30.124	11.287	1.00 16.91	E
ATOM	4626	CG	ARG	E	29	86.433	30.817	10.810	1.00 17.70	E
ATOM	4627	CD	ARG	B	29	86.791	32.117	10.109	1.00 18.98	E
ATOM	4628	NE	ARG	E	29	85.631	32.902	9.705	1.00 20.82	E
ATOM	4629	CZ	ARG		29	84.939	32.704	8.586	1.00 22.76	E
			ARG		29	85.285	31.739	7.743	1.00 21.05	E
MOTA	4630							8.309	1.00 20.13	E
ATOM	4631		ARC		29	83.904	33.482			E
MOTA	4632	C	ARG		29	88.842	28.435	12.710	1.00 18.44	
ATOM	4633	0	ARG	E	29	89.401	29.171	13.520	1.00 19.35	E
MOTA	4634	N	SEF	ξE	30	89.351	27.269	12.315	1.00 18.98	E
ATOM	4635	CA	SEE	RΕ	30	90.657	26.788	12.774	1.00 21.70	E
ATOM	4636	СВ		RE	30	90.619	25.284	13.028	1.00 22.10	E
					30	89.718	24.969	14.072	1.00 27.24	E
MOTA	4637	OG		RE			27.119	11.639	1.00 23.03	E
MOTA	4638	C		RE	30	91.637				E
MOTA	4639	0	SE	RE	30	91.509	26.604	10.528	1.00 23.56	
ATOM	4640	N	IL	B	31	92.611	27.978	11.927	1.00 23.05	E
MOTA	4641	CA	IL	EE	31	93.560	28.439	10.923	1.00 22.24	E
ATOM	4642	CB		EB	31	93.563	29.997	10.856	1.00 22.84	E
ATOM	4643		2 IL		31	94.163	30.470	9.545	1.00 19.19	E
			l IL			92.143	30.546	11.043	1.00 24.76	E
ATOM	4644						30.032	10.047	1.00 29.25	E
MOTA	4645		ı IL			91.144			1.00 24.53	E
MOTA	4646	С	IL	B E		95.013	28.014	11.134		
MOTA	4647	0	IL	EE		95.566	28.187	12.225	1.00 22.94	E
ATOM	4648		TY.	R E	32	95.625	27.468	10.081	1.00 24.41	E
ATOM	4649			RE		97.030	27.089	10.120	1.00 24.27	E
ATOM	4650			R E		97.277	25.755	9.417	1.00 26.61	E
				RE		98.733	25.338	9.444	1.00 29.24	E
MOTA	4651					99.423	25.231	10.649	1.00 30.69	B
MOTA	4652		l TY						1.00 32.83	E
MOTA	4653		1 TY			100.770		10.683		B
MOTA	4654		2 TY			99.426		8.267	1.00 31.46	
MOTA	4655	CE	2 TY	R E	32	100.774		8.288	1.00 32.58	E
MOTA	4656			R E		101.438	24.625	9.497		E
ATOM	4657			RE		102.768	24.280	9.522	1.00 33.44	E
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MOTA	4658	C	TYR	B	32	97.700	28.225	9.353	1.00 24.83	E
MOTA	4659	0	TYR		32	97.444	28.415	8.164	1.00 25.49	e
MOTA	4660	N	asn asn		33 33	98.543 99.202	28.985 30.146	10.045 9.461	1.00 24.28 1.00 24.25	E
ATOM ATOM	4661 4662	CA CB	ASN		33	100.144	29.740	8.324	1.00 23.93	B
ATOM	4663	CG	ASN		33	101.379	29.014	8.834	1.00 25.26	B
ATOM	4664	OD1	asn	B	33	102.003	29.439	9.808	1.00 26.40	B
MOTA	4665		asn		33	101.737	27.918	8.181	1.00 25.47	E
ATOM	4666	C	ASN		33	98.114 97.494	31.099 31.780	8.980 9.799	1.00 24.88 1.00 25.88	e
ATOM	4667 4668	N O	asn arg		33 34	97.494	31.760	7.677	1.00 24.52	E
MOTA MOTA	4669	CA	ARG		34	96.815	32.055	7.194	1.00 26.32	E
ATOM	4670	СВ	ARG		34	97.385	33.175	6.317	1.00 26.61	E
MOTA	4671	CG	ARG		34	97.999	34.346	7.072	1.00 26.37	E
MOTA	4672	CD	ARG		34	97.776	35.646	6.304	1.00 28.18 1.00 31.86	e
ATOM	4673	NE	ARG		34 34	97.886 97.607	35.429 36.332	4.865 3.931	1.00 31.88	E
ATOM ATOM	4674 4675	CZ	ARG		34	97.197	37.550	4.265	1.00 35.40	E
ATOM	4676		ARG		34	97.722	36.003	2.653	1.00 35.29	B
MOTA	4677	C	ARG	E	34	95.728	31.333	6.417	1.00 26.98	E
MOTA	4678	0	ARG		34	94.896	31.968	5.763	1.00 28.88	e
MOTA	4679	N	GLU		35	95.719 94.698	30.010 29.279	6.481 5.759	1.00 26.13 1.00 27.02	E
MOTA MOTA	4680 4681	CA CB	GLU		35 35	95.350	28.359	4.720	1.00 31.96	E
ATOM	4682	CG	GLU		35	96.284	27.301	5.278	1.00 38.52	E
ATOM	4683	CD	GLU		35	97.116	26.633	4.192	1.00 42.24	E
ATOM	4684		GLU		35	98.180	27.187	3.832	1.00 44.86	E
MOTA	4685	OE2			35	96.699	25.565	3.690 6.671	1.00 43.70 1.00 25.31	e
MOTA MOTA	4686	0	GLU		35 35	93.754 94.175	28.498 27.709	7.522	1.00 22.18	E
MOTA	4687 4688	N	GLU		36	92.464	28.756	6.498	1.00 24.46	E
ATOM	4689	CA	GLU		36	91.438	28.085	7.272	1.00 24.13	E
MOTA	4690	CB	GLU	E	36	90.085	28.731	7.001	1.00 24.37	E
MOTA	4691	CG	GLU		36	88.975	28.295	7.928	1.00 25.26 1.00 26.01	E
ATOM	4692	CD	GLU GLU		36 36	87.669 87.672	28.991 29.847	7.604 6.694	1.00 27.25	E
ATOM ATOM	4693 4694		GLU		36	86.646	28.689	8.253	1.00 27.12	E
ATOM	4695	c	GLU		36	91.413	26.630	6.826	1.00 23.40	B
MOTA	4696	0	GLU	JE	36	91.252	26.347	5.645	1.00 23.72	E
MOTA	4697	N	ILE		37	91.576	25.707	7.767	1.00 23.97 1.00 24.33	e E
ATOM	4698	CA	ILE		37	91.579 92.818	24.294 23.578	7.419 8.019	1.00 24.33	E
MOTA MOTA	4699 4700	CB	ILI LLI		37 37	94.096	24.255	7.532	1.00 24.26	E
ATOM	4701		ILI		37	92.771	23.616	9.544	1.00 25.10	B
MOTA	4702		LIL		37	93.822	22.742	10.204	1.00 26.49	E
MOTA	4703	C		E	37	90.301	23.555	7.836	1.00 23.49	E
MOTA	4704	0		3 B	37	89.871 89.690	22.627 23.975	7.162 8.936	1.00 23.62 1.00 25.16	E
ATOM ATOM	4705 4706	n Ca	VAI		38 38	88.465	23.342	9.415	1.00 25.85	E
ATOM	4707	CB		LE	38	88.715	22.489	10.667	1.00 26.44	E
MOTA	4708		L VA		38	87.516	21.610	10.932	1.00 27.10	E
ATOM	4709	CG:	2 VA		38	89.980	21.671	10.495	1.00 29.59	E
MOTA	4710	C		LE	38	87.481 87.885	24.428 25.471	9.792 10.288	1.00 24.45 1.00 24.36	E
MOTA MOTA	4711 4712	Ŋ		G B	38 39	86.193	24.168		1.00 24.90	E
ATOM	4713	CA		G E	39	85.175	25.161		1.00 23.66	B
MOTA	4714	CB	AR	G E	39	84.975	26.055		1.00 25.55	E
MOTA	4715	CG		g e		83.956			1.00 29.11 1.00 29.37	e
MOTA	4716	CD.		GE		83.514 84.626			1.00 29.70	E
MOTA MOTA	4717 4718	NE CZ		G E	•	84.505			1.00 31.37	E
MOTA	4719		1 AR			83.314			1.00 33.54	E
ATOM	4720		2 AR			85.572				E
MOTA	4721			G E		83.813			1.00 23.51	E
ATOM	4722			GE		83.385 83.147			1.00 23.83 1.00 22.04	B
MOTA MOTA	4723 4724			e e e e		81.799				E
MOTA	4725			EE		81.682			1.00 21.36	E
ATOM	4726	CG	PH	E	40	80.296				E
MOTA	4727		1 PE			79.944				e
MOTA	4728		2 PE			79.315 78.628				E
MOTA MOTA	4729		1 PH 2 PH			78.00				E
MOTA	4730 4731			ie i		77.66				E
		_	_							

MOTA	4732	C	PHE	E	40	80.938	26.148	11.395	1.00 21.77	B
ATOM	4733	0	DHR	B	40	81.064	27.167	12.071	1.00 20.81	E
MOTA	4734	N	ASP	B	41	80.067	26.033	10.404	1.00 21.82	E
MOTA	4735	CA	ASP		41	79.181	27.110	9.995	1.00 21.76	E
								8.470	1.00 22.62	B
MOTA	4736	CB	asp		41	79.190	27.182			
MOTA	4737	CG	ASP	E	41	78.492	28.400	7.929	1.00 23.09	E
ATOM	4738	OD1	ASP	E	41	77.507	28.864	8.546	1.00 22.57	E
ATOM	4739	OD2	ASP		41	78.929	28.881	6.861	1.00 25.40	E
										E
MOTA	4740	С	ASP		41	77.801	26.713	10.493	1.00 21.43	
MOTA	4741	0	ASP	E	41	77.277	25.672	10.085	1.00 22.83	E
MOTA	4742	N	SER	E	42	77.210	27.520	11.369	1.00 19.04	B
ATOM	4743	CA	SER		42	75.896	27.173	11.895	1.00 20.39	B
							28.220	12.907	1.00 19.13	E
ATOM	4744	CB	SER		42	75.399				
MOTA	4745	OG	SER	E	42	75.271	29.505	12.323	1.00 24.30	E
ATOM	4746	C	SER	E	42	74.891	27.000	10.762	1.00 20.23	E
ATOM	4747	0	SER	ĸ	42	73.916	26.267	10.910	1.00 18.97	E
	4748	N	ASP		43	75.145	27.660	9.631	1.00 21.77	E
ATOM										B
ATOM	4749	CA.	ASP		43	74.261	27.556	8.470	1.00 24.99	
ATOM	4750	CB	ASP	В	43	74.561	28.651	7.439	1.00 26.10	E
ATOM	4751	CG	ASP	B	43	73.819	29.947	7.727	1.00 28.71	E
ATOM	4752		ASP		43	73.078	30.013	8.737	1.00 28.83	E
										E
MOTA	4753		ASP		43	73.976	30.902	6.939	1.00 31.35	
MOTA	4754	C	ASP	E	43	74.378	26.193	7.809	1.00 25.68	E
ATOM	4755	0	ASP	E	43	73.424	25.727	7.190	1.00 28.27	B
ATOM	4756	N	VAL		44	75.544	25.558	7.937	1.00 25.47	B
							24.229	7.362	1.00 23.51	E
ATOM	4757	CA	VAL		44	75.764				
MOTA	4758	CB	VAL	B	44	77.251	24.007	6.964	1.00 24.39	E
ATOM	4759	CG1	VAL	E	44	77.456	22.579	6.491	1.00 19.52	E
ATOM	4760	CGS	VAL	E	44	77.655	24.984	5.867	1.00 23.79	B
							23.154	8.373	1.00 23.25	E
MOTA	4761	C	VAL		44	75.356				
MOTA	4762	0	VAL	E	44	74.774	22.136	8.005	1.00 22.01	E
MOTA	4763	N	GLY	E	45	75.683	23.370	9.644	1.00 22.52	E
ATOM	4764	CA	GLY	E	45	75.292	22.411	10.664	1.00 21.82	E
		c	GLY		45	76.275	21.311	11.001	1.00 22.07	E
MOTA	4765									E
MOTA	4766	0	GLY		45	75.982	20.442	11.818	1.00 22.49	
MOTA	4767	N	GLU	B	46	77.439	21.317	10.373	1.00 22.18	B
ATOM	4768	CA	GLU	E	46	78.421	20.295	10.691	1.00 23.77	E
MOTA	4769	CB	GLU		46	78.147	19.017	9.891	1.00 26.29	E
							19.112	8.411	1.00 28.23	E
MOTA	4770	CG	GLU		46	78.455				
MOTA	4771	æ	GLU	E	46	78.214	17.795	7.677	1.00 32.67	E
ATOM	4772	OE1	GLU	E	46	78.575	17.706	6.482	1.00 33.19	B
ATOM	4773	OE2			46	77.661	16.855	8.290	1.00 33.19	E
			GLU		46	79.807	20.839	10.383	1.00 23.15	E
ATOM	4774	C								E
ATOM	4775	0	GLU	E	46	79.943	21.880	9.747	1.00 23.06	
ATOM	4776	N	PHE	E	47	80.835	20.153	10.857	1.00 21.79	E
ATOM	4777	CA	PHE	E	47	82.192	20.595	10.599	1.00 22.22	E
		СВ	PHB		47	83.175	19.864	11.515	1.00 22.30	E
ATOM	4778								1.00 22.20	E
ATOM	4779	CG	PHE		47	83.058	20.249	12.968		
ATOM	4780	CD1	PHE	E	47	83.867	21.246	13.508	1.00 19.80	E
MOTA	4781	CD2	PHE	E	47	82.151	19.598	13.802	1.00 23.06	B
ATOM	4782		PHE		47	83.781	21.585	14.858	1.00 18.93	E
			PHE		47	82.055	19.931	15.157	1.00 22.63	E
ATOM	4783								1.00 20.81	
MOTA	4784	CZ	PHE		47	82.872	20.925	15.684		E
MOTA	4785	C	PHE	E	47	82.513	20.278	9.147	1.00 24.14	E
MOTA	4786	0	PHE	E	47	82.064	19.258	8.609	1.00 23.25	E
ATOM	4787	N	ARG		48	83.272	21.164	8.511	1.00 22.66	E
						83.672	20.966	7.131	1.00 23.86	B
MOTA	4788	CA	ARG		48					
MOTA	4789	CB	ARG	E	48	82.801	21.795	6.181	1.00 23.48	E
MOTA	4790	CG	ARG	Ε	48	81.339	21.375	6.091	1.00 25.01	B
ATOM	4791	CD	ARG	E	48	81.155	20.061	5.348	1.00 25.08	E
		NE	ARG		48	79.747	19.811	5.044	1.00 27.17	E
MOTA	4792							4.164	1.00 29.38	E
MOTA	4793	CZ	ARC		48	79.038	20.515			
MOTA	4794		ARG		48	79.604	21.513	3.498	1.00 31.36	E
ATOM	4795	NH	ARG	B	48	77.763	20.226	3.946	1.00 30.50	E
ATOM	4796	C	ARG		48	85.119	21.395	6.972	1.00 24.13	E
			ARG		48	85.507	22.480	7.416	1.00 25.58	B
MOTA	4797	0							1.00 22.26	E
MOTA	4798	N	ALA		49	85.924	20.537	6.360		
MOTA	4799	CA	ALF		49	87.316	20.875	6.122	1.00 23.11	E
MOTA	4800	CB	AL/	E	49	88.102	19.630	5.711	1.00 22.46	E,
MOTA	4801		ALA		49	87.290	21.875	4.980	1.00 22.04	E
			AL		49	86.507	21.722	4.048	1.00 23.16	E
ATOM	4802								1.00 23.56	E
MOTA	4803	N	VAI		50	88.108	22.916	5.050		
ATOM	4804	CA	VAI	E	50	88.135	23.875		1.00 23.79	E
ATOM	4805		VAI	B	50	88.059	25.360	4.478	1.00 24.14	E
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ATOM	4806	CG1	VAL	B	50	88.341	25.408	5.959	1.00 24.71	E
ATOM	4807	CG2	VAL	E	50	89.010	26.268	3.704	1.00 22.47	B
ATOM	4808	С	VAL	E	50	89.374	23.578	3.098	1.00 23.50	B
MOTA	4809	ō	VAL		50	89.485	24.041	1.963	1.00 24.92	B
		N	THR		51	90.281	22.770	3.650	1.00 24.49	E
ATOM	4810								1.00 25.50	E
MOTA	4811	CA	THR		51	91.492	22.317	2.951		
MOTA	4812	CB	THR		51	92.742	23.198	3.234	1.00 25.69	E
MOTA	4813	OG1	THR	E	51	93.171	23.007	4.586	1.00 27.89	E
MOTA	4814	CG2	THR	E	51	92.443	24.670	2.985	1.00 23.29	B
MOTA	4815	C	THR	E	51	91.817	20.895	3.420	1.00 26.59	B
MOTA	4816	0	THR		51	91.387	20.477	4.496	1.00 27.35	E
		N	LEU		52	92.576	20.154	2.617	1.00 28.03	E
ATOM	4817						18.783		1.00 28.49	E
MOTA	4818	CA	LEU		52	92.949		2.956		
MOTA	4819	CB	TEO		52	93.995		1.969	1.00 30.33	E
MOTA	4820	CG	FEA	E	52	93.536	17.892	0.556	1.00 34.17	E
ATOM	4821	CD1	LEU	E	52	94.749	17.628	-0.334	1.00 34.41	E
ATOM	4822	CD2	LEU	B	52	92.644	16.668	0.620	1.00 34.30	E
ATOM	4823	C	LEU	B	52	93.494	18.645	4.374	1.00 28.20	E
MOTA	4824	0	LEU		52	93.304	17.624	5.027	1.00 29.17	E
ATOM	4825	N	LEU		53	94.179	19.677	4.839	1.00 28.30	E
						94.766	19.682	6.171	1.00 28.75	B
MOTA	4826	CA	LEU		53					
MOTA	4827	CB	LEU		53	95.490	21.015	6.387	1.00 30.37	E
ATOM	4828	CG	LEU	B	53	96.939	21.010	6.882	1.00 32.74	E
ATOM	4829	CD1	LEU	E	53	97.77 <i>7</i>	20.085	6.008	1.00 31.60	E
ATOM	4830	CD2	LEU	K	53	97.498	22.444	6.854	1.00 30.06	E
ATOM	4831	C	LEU		53	93.727	19.464	7.278	1.00 27.82	E
MOTA	4832	ō	LEU		53	94.027	18.858	8.312	1.00 25.47	B
					54	92.508	19.957	7.059	1.00 27.39	E
ATOM	4833	N	GLY						1.00 26.92	8
MOTA	4834	CA	GLX		54	91.466	19.813	8.062		
ATOM	4835	C	GLY	E	54	90.569	18.589	7.949	1.00 28.33	E
ATOM	4836	0	GLY	B	54	89.725	18.348	8.813	1.00 28.02	B
ATOM	4837	N	LEU	B	55	90.755	17.801	6.898	1.00 29.28	E
ATOM	4838	CA	LEU	E	55	89.930	16.620	6.675	1.00 31.43	E
MOTA	4839	CB	LEU		55	90.410	15.885	5.419	1.00 32.39	E
	4840	CG	LEU		55	89.426	14.934	4.731	1.00 35.68	E
MOTA								4.504	1.00 34.41	B
MOTA	4841		LEU		55	88.086	15.627			E
MOTA	4842		LEU		55	90.018	14.473	3.406	1.00 35.99	
MOTA	4843	C	PEA	B	55	89.865	15.659	7.867	1.00 32.09	E
MOTA	4844	0	LEU	E	55	88.778	15.294	8.312	1.00 32.58	B
ATOM	4845	N	PRO	E	56	91.023	15.235	8.402	1.00 31.67	E
MOTA	4846	CD	PRO	E	56	92.411	15.520	8.000	1.00 31.37	E
ATOM	4847	CA	PRO		56	90.986	14.316	9.546	1.00 31.17	E
	4848	СВ	PRO		56	92.459	14.163	9.919	1.00 30.50	B
ATOM						93.161	14.352	8.611	1.00 31.19	E
ATOM	4849	CG	PRO		56					E
MOTA	4850	C	PRO		56	90.158	14.865	10.708	1.00 31.43	
MOTA	4851	0	PRO		56	89.250	14.195	11.205	1.00 32.17	E
ATOM	4852	N	ALA	E	57	90.473	16.086	11.138	1.00 29.94	B
MOTA	4853	CA	ALA	E	57	89.748	16.709	12.244	1.00 28.45	E
ATOM	4854	CB	ALA	E	57	90.314	18.098	12.532	1.00 27.09	E
ATOM	4855	C	ALA		57	88.249	16.807	11.960	1.00 27.57	E
ATOM	4856	ō	ALA		57	87.436	16.466	12.812	1.00 26.57	E
					58	87.899	17.270	10.761	1.00 27.40	E
MOTA	4857	N	ALA						1.00 28.85	E
MOTA	4858	CA	ALA		58	86.505	17.422	10.349		
MOTA	4859	CB	ALA		58	86.439	18.007	8.939	1.00 27.80	E
ATOM	4860	C	ALA	. B	58	85.726	16.110	10,406	1.00 30.37	E
ATOM	4861	0	ALA	E	58	84.624	16.058	10.954	1.00 29.58	B
ATOM	4862	N	GLU	E	59	86.292	15.052	9.837	1.00 32.24	E
ATOM	4863	CA	GLU		59	85.632	13.750	9.845	1.00 35.22	E
ATOM	4864	CB	GLU		59	86.441	12.724	9.049	1.00 36.81	E
			GLU		59	86.392	12.917	7.549	1.00 40.89	. E
ATOM	4865	CG							1.00 44.28	E
ATOM	4866	CD	GLU		59	87.057	11.775	6.805		
ATOM	4867		. GLU		59	88.291	11.597	6.955	1.00 45.76	E
MOTA	4868	OE2	GLU	E	59	86.342	11.052	6.075	1.00 45.12	B
MOTA	4869	C	GLU	E	59	85.441	13.231	11.260	1.00 34.08	B
ATOM	4870	0	GLU	ΙE	59	84.384	12.697	11.596	1.00 34.48	E
ATOM	4871	N	TYR		60	86.466	13.387	12.090	1.00 33.21	B
	4872	CA	TYR		60	86.390	12.919	13.463	1.00 32.36	B
MOTA			TYR		60	87.724	13.101	14.177	1.00 33.78	B
ATOM	4873	CB						15.594	1.00 35.68	E
MOTA	4874	CG	TYR		60	87.657	12.617			
MOTA	4875		TYF		60	87.543	11.259	15.872	1.00 37.48	E
ATOM	4876		TYF		60	87.394	10.802	17.173	1.00 41.14	E
MOTA	4877	CD2	TYF	E	60	87.628	13.514	16.655	1.00 37.26	E
ATOM	4878	CE2	TYF	E	60	87.478	13.073	17.965	1.00 40.26	E
ATOM	4879	CZ	TYF		60	87.360	11.714	18.218	1.00 41.88	E

ATOM	4880	OH	TYR	E	60	87.198	11.262	19.508	1.00 44.51	E
MOTA	4881	C	TYR		60	85.312	13.623	14.275	1.00 32.30	E
ATOM	4882	0	TYR		60	84.430	12.976	14.839	1.00 30.56	E
MOTA	4883	N	TRP TRP		61	85.391	14.950 15.715	14.347 15.112	1.00 31.42 1.00 31.35	e
MOTA MOTA	4884 4885	CA CB	TRP		61 61	84.412 84.744	17.219	15.071	1.00 32.78	E
ATOM	4886	CG	TRP		61	86.051	17.584	15.748	1.00 35.14	E
ATOM	4887		TRP		61	86.909	18.687	15.425	1.00 37.07	E
ATOM	4888	CE2	TRP		61	87.994	18.655	16.331	1.00 37.15	E
MOTA	4889	CE3	TRP		61	86.864	19.706	14.458	1.00 39.50	E
ATOM	4890	CD1	TRP	E	61	86.635	16.947	16.809	1.00 35.82	E
MOTA	4891	NB1	TRP	E	61	87.800	17.582	17.163	1.00 35.66	B
MOTA	4892	CZ2	TRP		61	89.034	19.602	16.300	1.00 38.95	E
ATOM	4893	CZ3	TRP		61	87.902	20.656	14.427	1.00 41.16	B
ATOM	4894	CH2			61	88.971	20.591	15.346 14.653	1.00 40.81 1.00 29.29	E
ATOM ATOM	4895 4896	С 0	TRP		61 61	82.968 82.045	15.472 15.563	15.458	1.00 29.20	E
ATOM	4897	N	ASN		62	82.772	15.162	13.373	1.00 27.86	E
ATOM	4898	CA	ASN		62	81.428	14.902	12.853	1.00 29.09	E
ATOM	4899	CB	ASN		62	81.379	15.051	11.331	1.00 29.42	E
MOTA	4900	CG	asn	E	62	81.241	16.492	10.893	1.00 31.22	B
ATOM	4901		asn		62	80.563	17.288	11.545	1.00 29.56	E
ATOM	4902		asn		62	81.870	16.834	9.772	1.00 31.73	E
ATOM	4903	C	ASN		62	80.906	13.519	13.220	1.00 28.26	E
ATOM	4904	0	ASN		62	79.716	13.242	13.086	1.00 27.48 1.00 27.47	e
ATOM ATOM	4905	N	SER SER		63 63	81.795 81.381	12.647 11.311	13.672 14.056	1.00 27.47	E
ATOM	4906 4907	CA CB	SER		63	82.511	10.310	13.803	1.00 28.56	E
ATOM	4908	OG	SER		63	83.607	10.545	14.671	1.00 32.72	B
ATOM	4909	c	SER		63	80.987	11.310	15.534	1.00 30.11	E
ATOM	4910	ō	SER		63	80.515	10.297	16.055	1.00 31.52	E
ATOM	4911	N	GLN	E	64	81.173	12.453	16.196	1.00 28.86	E
MOTA	4912	CA	GLN		64	80.834	12.604	17.612	1.00 28.28	E
ATOM	4913	CB	GLN		64	81.929	13.379	18.350	1.00 29.50	E
MOTA	4914	CG	GLM		64	83.330	12.787	18.266	1.00 29.72	e
ATOM	4915	CD CD	GLN		64 64	83.418 83.055	11.412 10.405	18.888 18.267	1.00 32.69 1.00 35.22	E
MOTA MOTA	4916 4917	OE1 NE2			64	83.887	11.358	20.128	1.00 31.92	E
ATOM	4918	C	GLN		64	79.522	13.366	17.783	1.00 28.42	E
ATOM	4919	ō	GLN		64	79.525	14.599	17.800	1.00 27.68	B
ATOM	4920	N	LYS		65	78.410	12.648	17.926	1.00 27.17	E
MOTA	4921	CA	LYS	E	65	77.111	13.300	18.097	1.00 29.82	E
MOTA	4922	CB	LYS	E	65	75.994	12.258	18.253	1.00 31.43	B
MOTA	4923	CG	LYS		65	75.479	11.692	16.936	1.00 37.61	E
ATOM	4924	CD	LYS		65	74.801	12.766	16.072	1.00 41.12	E
MOTA	4925	CE	LYS		65	73.489	13.267	16.696	1.00 44.25 1.00 44.10	E
MOTA	4926 4927	NZ C	LYS		65 65	72.832 77.067	14.322 14.273	15.861 19.278	1.00 28.07	E
ATOM ATOM	4928	o	LYS		65	76.406	15.308	19.211	1.00 27.46	E
ATOM	4929	N	ASP		66	77.758	13.938	20.361	1.00 27.40	E
ATOM	4930	CA	ASP		66	77.783	14.809	21.532	1.00 26.85	E
ATOM	4931	CB	ASP	B	66	78.566	14.142	22.670	1.00 26.10	E
MOTA	4932	CG	ASP		66	79.899	13.576	22.212	1.00 29.25	E
MOTA	4933		ASP		66	79.915	12.836	21.205	1.00 28.95	B
MOTA	4934		ASP		66	80.929	13.858	22.864	1.00 31.03 1.00 26.21	e
MOTA	4935	C	ASP ASP		66 66	78.390 77.844	16.174 17.215	21.193 21.559	1.00 26.58	E
MOTA MOTA	4936 4937	N O	ILE		67	79.510	16.170	20.478	1.00 26.25	E
MOTA	4938	CA	ILB		67	80.164	17.414	20.100	1.00 25.76	E
ATOM	4939	CB	ILE		67	81.551	17.153	19.477	1.00 27.31	E
ATOM	4940	CG2	ILE	E	67	82.261	18.467	19.210	1.00 25.90	E
MOTA	4941	CG1	. ILE	E	67	82.396	16.304	20.429	1.00 28.85	E
MOTA	4942	CD1	. ILE		67	82.494	16.871	21.844	1.00 32.35	E
MOTA	4943	C	ILE		67	79.307	18.189	19.108	1.00 25.95	E
ATOM	4944	0	ILE		67	79.125	19.392	19.255	1.00 26.97 1.00 26.05	e
MOTA	. 4945	N	LEU		68 68	78.775	17.504 18.172	18.100 17.113	1.00 26.05	E
MOTA MOTA	4946 4947	CA CB	LEU		68 68	77.927 77.382	17.169	16.094	1.00 26.36	E
MOTA	4947	CG	LEU		68	78.154	16.987	14.790	1.00 27.01	E
MOTA	4949		LEU		68	77.389	16.002	13.913	1.00 26.26	E
ATOM	4950		LEU		68	78.311	18.342	14.076	1.00 24.04	E
ATOM	4951	C	LEU	E	68	76.760	18.870	17.792	1.00 26.03	E
MOTA	4952	0	LEU		68	76.433	20.011	17.465	1.00 25.76	E
MOTA	4953	N	GLU	E	69	76.134	18.175	18.737	1.00 27.50	E

75.000 18.726 19.471 1.00 30.38 ATOM 4954 CA GLU E 69 ATOM 4955 CB GLU E 69 74.481 17.720 20.508 1.00 34.06 E ATOM 4956 CG GLU E 69 73.426 16.742 19.989 1.00 40.55 ATOM 4957 CD GLUE 69 72.211 17.444 19.392 1.00 44.43 ATOM 4958 OB1 GLU E 69 71.802 18.505 19.922 1.00 43.73 ATOM 4959 71.656 16.926 OB2 GLU E 69 18.397 1.00 48.15 ATOM 4960 С GLU E 69 75.335 20.034 20.178 1.00 29.17 ATOM 74.587 21.009 4961 0 GLU E 69 20.071 1.00 29.71 ATOM 4962 N ARG E 70 76.453 20.059 20.899 1.00 26.65 76.844 21.262 ATOM 4963 CA ARG E 70 21.620 1.00 25.51 MOTA 4964 CB ARG E 70 78.001 20.965 22.572 1.00 27.14 В ATOM 4965 CG ARG B 70 77.711 19.855 23.563 1.00 31.22 E ATOM 4966 CD ARG E 70 78.637 19.934 24.769 1.00 35.11 NE ARGE 78.758 18.647 ATOM 4967 70 25.440 1.00 39.19 R CZ ARG E 70 79.456 17.628 ATOM 4968 24.956 1.00 41.08 R MOTA 4969 NH1 ARG E 70 80.096 17.752 23.802 1.00 45.32 ATOM 4970 NH2 ARG E 70 79.511 16.486 25.618 1.00 44.01 ATOM 4971 C ARG E 70 77.230 22.395 20.677 1.00 24.57 B 76.927 23.557 77.897 22.057 ATOM 4972 ARG E 70 20.941 1.00 21.44 0 B ATOM 4973 N LYS E 71 19.576 1.00 24.56 В ATOM 4974 CA LYS E 71 78.309 23.071 18.612 1.00 24.08 ATOM 4975 CB LYS E 71 79.202 22.452 17.534 1.00 25.39 B ATOM CG LYS E 71 80.100 23.474 4976 16.852 1.00 29.73 ĸ ATOM 4977 CD LYS E 71 81.067 24.095 17.862 1.00 30.94 ATOM 4978 CE LYS E 71 81.905 25.205 17.256 1.00 31.82 ATOM 4979 NZ LYS E 71 82.774 25.849 18.290 1.00 33.45 B 77.087 23.732 77.045 24.951 MOTA 4980 C LYS E 71 17.960 1.00 22.42 R ATOM 4981 0 LYS E 71 17.780 1.00 18.65 В ATOM 4982 N ARG E 72 76.092 22.919 17.620 1.00 22.31 ATOM 4983 CA ARG E 72 74.867 23.419 17.002 1.00 21.44 R CB ARG E 72 73.984 22.250 ATOM 16.578 1.00 19.93 4984 R ATOM 4985 CG ARG E 72 74.534 21.497 15.407 1.00 21.45 MOTA 4986 CD ARG E 72 73.779 20.223 15.141 1.00 23.34 MOTA 4987 NE ARGE 72 74.211 19.643 13.877 1.00 24.99 Е CZ ARG E 72 74.028 18.377 ATOM 13.522 1.00 27.42 4988 E NH1 ARG E 72 ATOM 4989 73.411 17.533 14.344 1.00 25.90 E ATOM 4990 NH2 ARG E 72 74.475 17.955 12.341 1.00 25.41 74.093 24.315 ATOM 4991 С ARG E 72 17.961 1.00 21.34 ARG E 72 73.336 25.182 MOTA 4992 0 17.535 1.00 23.67 R ALA E 73 74.293 24.105 19.256 1.00 21.13 ATOM 4993 N MOTA 4994 CA ALA E 73 73.610 24.887 20.281 1.00 22.11 CB ALA E 73 MOTA 4995 73.476 24.052 21.568 1.00 21.20 ALA E 73 20.576 1.00 22.67 MOTA 4996 C 74.347 26.189 E ALA B 73 73.773 27.133 MOTA 4997 0 21.125 1.00 25.58 Е MOTA 4998 N ALA E 74 75.614 26.248 20.195 1.00 22.52 76.420 27.432 20.448 MOTA 4999 CA ALA B 74 1.00 22.20 ATOM 5000 CB ALA E 74 77.830 27.219 19.910 1.00 24.81 5001 ALA E 74 75.828 28.722 19.882 1.00 22.28 MOTA C E MOTA 5002 0 ALA E 74 76.027 29.796 20.452 1.00 20.24 E VAL B 75 MOTA 5003 N 75.102 28.634 18.770 1.00 21.92 CA VAL B 75 74.519 29.841 18.185 1.00 21.69 ATOM 5004 E CB VAL E 75 73.700 29.517 MOTA 5005 16.890 1.00 22.61 E ATOM 5006 CG1 VAL E 75 72.488 28.657 17.219 1.00 24.39 MOTA 5007 CG2 VAL E 75 73.270 30.798 16.218 1.00 24.00 E MOTA 5008 C VAL E 75 73.639 30.558 19.219 1.00 21.26 E 5009 VAL E 75 MOTA 0 73.464 31.777 19.164 1.00 20.64 MOTA 5010 N ASP E 76 73.106 29.802 20.171 1.00 20.84 MOTA 5011 CA ASP E 76 72.273 30.385 21.220 1.00 23.98 CB ASP E 76 MOTA 5012 71.022 29.532 21.471 1.00 25.33 Е MOTA 5013 CG ASP E 76 70.010 29.605 20.331 1.00 27.46 E MOTA 50,14 OD1 ASP B 76 69.807 30.697 19.763 1.00 29.45 5015 OD2 ASP E MOTA 76 69.398 28.566 20.020 1.00 31.17 5016 ASP E 73.044 30.525 22.538 MOTA С 76 1.00 24.46 ASP E 76 72.910 MOTA 5017 0 31.524 23.247 1.00 25.64 R MOTA 5018 N ARG E 77 73.846 29.515 22.855 1.00 23.56 E MOTA 5019 CA ARG E 77 74.627 29.486 24.085 1.00 22.99 MOTA 5020 CB ARG E 75.176 28.077 24.279 1.00 26.55 77 ATOM 5021 CG ARG E 77 75.848 27.806 25.607 1.00 33.45 E ARG E 77 5022 MOTA CD 75.961 26.295 25.825 1.00 37.66 MOTA 5023 NE ARGE 77 74.639 25.666 25.883 1.00 40.99 CZ ARG E 77 ATOM 5024 74.423 24.352 25.862 1.00 43.13 ATOM 5025 NH1 ARG E 77 75.438 23.503 25.782 1.00 43.11 NH2 ARG E 77 25.914 1.00 44.93 ATOM 5026 73.183 23.885 С ARG R 77 ATOM 5027 75.763 30.509 24.078 1.00 23.23

ATOM 5028 O ARG E 77 76.162 31.022 25.129 1.00 23.14 R ATOM VAL E 78 5029 N 76.275 30.808 22.889 1.00 20.54 ATOM 5030 CA VAL E 78 77.354 31.767 22.741 1.00 19.56 ATOM 5031 CB VAL E 78 78.500 31.181 21.891 1.00 19.17 5032 CG1 VAL E 78 ATOM 79.612 32.208 21.724 1.00 17.69 ATOM 5033 CG2 VAL E 78 79.032 29.921 22.541 1.00 19.40 76.888 33.075 76.786 34.110 ATOM 5034 C VAL E 78 22.093 1.00 19.95 VALE 78 ATOM 5035 0 22.756 1.00 21.57 ATOM 5036 N CYS E 79 76.595 33.021 20.799 1.00 17.88 MOTA 5037 CA CYS E 79 76.181 34.205 20.059 1.00 17.48 ATOM 5038 C CYS E 79 74.967 34.966 20,620 1.00 18.40 5039 O CYS E 79 5040 CB CYS E 79 ATOM 75.087 36.146 75.946 33.847 20.967 1.00 16.69 R MOTA 18.592 1.00 17.30 R ATOM 5041 SG CYS B 79 77.361 33.071 17.722 1.00 27.04 E 5042 N ARG E 80 5043 CA ARG E 80 MOTA 73.802 34.326 20.717 1.00 17.59 ATOM 72.641 35.050 21.240 1.00 20.01 E 5044 CB ARG E 80 ATOM 71.340 34.256 21.032 1.00 20.22 E 70.886 34.213 19.584 1.00 22.92 69.423 33.811 19.439 1.00 23.91 MOTA 5045 CG ARG E 80 ATOM 5046 CD ARG E 80 5047 NE ARG E 80 68.972 33.965 18.057 1.00 23.49 MOTA E ATOM CZ ARG E 80 69.206 33.089 17.082 1.00 25.16 E ATOM 5049 NH1 ARG B 80 69.884 31.975 17.326 1.00 24.15 68.778 33.336 15.851 1.00 25.51 72.804 35.423 22.716 1.00 20.35 MOTA 5050 NH2 ARG E 80 ATOM 5051 C ARG E 80 E 5052 O ARG E 80 72.317 36.464 23.153 1.00 17.98 MOTA R ATOM 5053 N HIS E 81 73.495 34.581 23.479 73.717 34.867 24.895 1.00 21.22 CA HIS E 81 ATOM 5054 1.00 22.79 ATOM CB HIS E 81 5055 74.467 33.717 25.572 1.00 24.38 ATOM CG HIS E 81 5056 74.955 34.046 26.950 1.00 26.42 CD2 HIS E 81 76.188 34.381 27.404 1.00 26.61 ATOM 5057 E ND1 HIS B 81 ATOM 5058 74.122 34.080 28.048 1.00 26.60 ATOM 5059 CE1 HIS B 81 74.819 34.420 29.117 1.00 25.75 E ATOM 5060 NE2 HIS E 81 76.075 34.609 28.754 1.00 26.16 E C HIS E 81 74.531 36.146 25.060 74.109 37.076 25.742 ATOM 5061 1.00 21.41 ATOM 5062 0 HIS B 81 1.00 19.84 N ASN E 82 CA ASN E 82 ATOM 5063 N 75.700 36.188 24.426 1.00 22.13 ATOM 5064 76.568 37.361 24.535 1.00 21.51 E ATOM 5065 CB ASN E 82 77.927 37.111 23.864 1.00 18.47 B CG ASN E 82 OD1 ASN E 82 ATOM 5066 78.702 35.982 24.515 1.00 18.09 ATOM. 5067 78.453 35.632 25.669 1.00 19.05 5068 ND2 ASN E 82 ATOM 79.656 35.409 23.777 1.00 15.06 75.936 38.612 23.949 1.00 20.33 76.212 39.716 24.412 1.00 22.84 ATOM 5069 C ASN E 82 1.00 20.33 ASN E 82 MOTA 5070 O TYR E 83 MOTA 5071 N 75.089 38.454 22.940 1.00 19.71 MOTA 5072 CA TYR E 83 74.454 39.620 22.336 1.00 20.96 73.619 39.211 21.114 1.00 21.58 MOTA 5073 CB TYR E 83 E MOTA 5074 CG TYR E 83 73.223 40.368 20.218 1.00 22.56 MOTA 5075 CD1 TYR E 83 72.047 41.090 20.439 1.00 23.70 5076 CE1 TYR E 83 MOTA 71.682 42.152 19.593 1.00 25.46 R 74.027 40.736 19.140 1.00 22.35 73.675 41.788 18.297 1.00 24.48 MOTA 5077 CD2 TYR E 83 5078 CE2 TYR E 83 ATOM 5079 CZ TYR E 83 ATOM 72.508 42.491 18.523 1.00 26.06 72.185 43.524 17.671 1.00 28.63 73.583 40.345 23.363 1.00 21.22 ATOM 5080 OH TYR E 83 R 5081 C ATOM TYR E 83 5082 O TYR E 83 ATOM 73.399 41.557 23.276 1.00 21.25 5083 N MOTA GLN E 84 73.046 39.606 24.333 1.00 22.94 MOTA 5084 CA GLN B 84 72.234 40.226 25.377 1.00 25.07 71.631 39.180 26.324 1.00 25.76 70.863 38.047 25.653 1.00 30.97 ATOM 5085 CB GLN B 84 ATOM 5086 CG GLN E 84 5087 CD GLN E 84 MOTA 69.889 38.525 24.594 1.00 33.95 ATOM 5088 OE1 GLN E 84 69.055 39.401 24.840 1.00 36.35 69.986 37.940 23.401 1.00 36.25 MOTA 5089 NE2 GLN E 84 ATOM GLN E 84 5090 C 73.158 41.145 26.174 1.00 25.41 ATOM 5091 0 GLN E 84 72.804 42.290 26.473 1.00 27.11 5092 N ATOM LEU E 85 74.344 40.637 26.510 1.00 24.17 75.330 41.413 27.256 1.00 26.47 76.601 40.590 27.515 1.00 26.91 ATOM 5093 CA LEU E 85 Е 5094 CB LEU E 85 ATOM ATOM 5095 CG LEU E 85 76.485 39.202 28.161 1.00 29.65 5096 CD1 LBU E 85 ATOM 77.872 38.735 28.587 1.00 31.29 MOTA 5097 CD2 LEU E 85 75.564 39.247 29.365 1.00 32.27 75.698 42.661 26.459 1.00 26.89 75.762 43.757 27.004 1.00 28.24 ATOM 5098 С LEU B 85 MOTA 5099 O LEU B 85 5100 N 5101 CA MOTA GLU E 86 75.941 42.484 25.162 1.00 27.39 ATOM GLU E 86 76.293 43.603 24.295 1.00 28.02

ATOM	5102	СВ	GLU	E	86	76.492	43.126	22.852	1.00 26.60	B
MOTA	5103	CG	GΓΩ	E	86	77.524	42.026	22.672	1.00 30.65	B
ATOM	5104	CD	GLU		86	78.942	42.457	23.024	1.00 31.17	E
MOTA	5105		GLU		86	79.860	41.612	22.919	1.00 31.68	E
ATOM	5106	OE2	GLU		86	79.139	43.631	23.402	1.00 31.77	B
ATOM	5107	C	GLU		86	75.165 75.407	44.630	24.327	1.00 27.95 1.00 24.30	e
MOTA	5108	0	GLU		86 87	75.407 73.935	45.834 44.130	24.257 24.442	1.00 24.30	E
ATOM ATOM	5109 5110	n Ca	LEU		87	72.736	44.962	24.468	1.00 32.20	E
ATOM	5111	CB	FEA		87	71.496	44.062	24.423	1.00 32.64	E
ATOM	5112	CG	LEU		87	70.506	44.100	23.248	1.00 35.59	B
ATOM	5113		LEU		87	71.101	44.734	21.997	1.00 35.24	E
ATOM	5114		LEU		87	70.071	42.675	22.965	1.00 34.35	E
MOTA	5115	C	LEU	B	87	72.669	45.893	25.686	1.00 33.33	E
ATOM	5116	0	LEU	B	87	71.967	46.902	25.663	1.00 32.52	E
MOTA	5117	N	ARG		88	73.401	45.560	26.745	1.00 35.06	E
ATOM	5118	CA	ARG		88	73.399	46.389	27.948	1.00 37.29	E
MOTA	5119	CB	ARG		88	73.348	45.524	29.215	1.00 39.69	E
MOTA	5120	CG	ARG		88	72.471	44.275	29.158	1.00 43.37 1.00 45.38	e
ATOM	5121	CD	ARG ARG		88 88	72.441 71.846	43.592 42.257	30.529 30.499	1.00 45.36	E
ATOM ATOM	5122 5123	NE CZ	ARG		88	70.625	41.985	30.047	1.00 50.95	E
ATOM	5124		ARG		88	69.854	42.958	29.579	1.00 52.23	E
ATOM	5125		ARG		88	70.171	40.738	30.064	1.00 51.26	E
ATOM	5126	C	ARG		88	74.670	47.225	28.010	1.00 37.36	E
ATOM	5127	0	ARG	E	88	74.842	48.044	28.913	1.00 37.55	E
ATOM	5128	N	THR	E	89	75.564	47.019	27.049	1.00 36.40	E
MOTA	5129	CA	THR	E	89	76.834	47.731	27.055	1.00 34.93	B
MOTA	5130	CB	THR	E	89	77.951	46.807	27.590	1.00 36.26	E
ATOM	5131	OG1	THR	E	89	77.973	45.590	26.825	1.00 34.21	E
ATOM	5132	CG2			89	77.708	46.478	29.056	1.00 33.95	E
MOTA	5133	С	THR		89	77.294	48.304	25.718	1.00 33.37	E
ATOM	5134	0	THR		89	76.958	49,431	25.356	1.00 33.30	E
MOTA	5135	N	THR		90	78.080	47.510	25.000	1.00 32.11	e
MOTA	5136	CA	THR		90	78.639 79.313	47.895 46.681	23.712 23.041	1.00 30.45 1.00 31.20	E
ATOM	5137	CB	THR		90 90	80.238	46.086	23.958	1.00 32.67	E
MOTA MOTA	5138 5139		THR		90	80.076	47.109	21.811	1.00 32.64	E
ATOM	5140	C	THR		90	77.639	48.504	22.738	1.00 28.40	E
ATOM	5141	Ö	THR		90	77.903	49.538	22.133	1.00 27.20	B
ATOM	5142	N	LEU		91	76.489	47.864	22.582	1.00 29.83	E
ATOM	5143	CA	LEU		91	75.482	48.361	21.655	1.00 29.52	E
ATOM	5144	CB	LEU	E	91	74.474	47.252	21.354	1.00 27.50	E
ATOM	5145	CG	LEU	E	91	75.091	46.101	20.550	1.00 26.15	E
MOTA	5146		LEU		91	74.102	44.959	20.457	1.00 24.51	B
ATOM	5147		LEU		91	75.487	46.593	19.157	1.00 23.04	E
MOTA	5148	C	LEU		91	74.770	49.629	22.129	1.00 30.74	B
MOTA	5149	0	LEU		91	73.994	50.228 50.043	21.382	1.00 31.46 1.00 29.33	E
MOTA	5150	N	GLN		92	75.035	51.259	23.366 23.884	1.00 30.04	E
MOTA MOTA	5151 5152	CA CB	GLN GLN		92 92	74.427 73.869	51.044	25.294	1.00 30.04	E
ATOM	5153	CG	GLN		92	72.500	50.381	25.327	1.00 36.90	E
MOTA	5154	CD	GLN		92	71.865	50.426	26.706	1.00 41.59	E
ATOM	5155		GLN		92	70.760	49.920	26.911	1.00 43.76	B
MOTA	5156		GLN		92	72.563	51.037	27.662	1.00 43.75	Œ
MOTA	5157	С	GLN	B	92	75.430	52.409	23.898	1.00 28.45	E
MOTA	5158	0	GLN	E	92	75.059	53.558	24.125	1.00 28.57	B
ATOM	5159	N	ARG	E	93	76.699	52.098	23.650	1.00 26.37	E
MOTA	5160	CA	ARG		93	77.737	53.127	23.633	1.00 26.74	E
MOTA	5161	CB	ARG		93	79.112	52.513	23.340	1.00 24.84	E
ATOM	5162	CG	ARG		93	80.260	53.525	23.217	1.00 20.15	B
ATOM	5163	CD	ARG		93	81.569	52.801	22.894	1.00 20.06 1.00 15.27	E
ATOM	5164	NE	ARG		93	82.718	53.685 54.330	22.729 23.729	1.00 15.27	B
MOTA MOTA	5165 5166	CZ	ARG L ARG		93 93	83.316 82.875	54.197	24.973	1.00 17.82	B
ATOM	5167		ARG		93 93	84.367	55.101	23.492	1.00 16.28	E
ATOM	5168	C	ARG		93	77.428	54.173	22.576	1.00 28.26	B
ATOM	5169	ō	ARG		93	77.202	53.847	21.407	1.00 29.80	E
ATOM	5170	N	ARG		94	77.411	55.431	22.995	1.00 28.24	B
ATOM	5171	CA	ARG		94	77.159	56.529	22.084	1.00 29.74	E
MOTA	5172	CB	ARG	E	94	75.661	56.855	22.053	1.00 32.88	E
MOTA	5173	CG	ARG		94	74.912	55.941	21.086	1.00 36.76	E
MOTA	5174	CD	ARG		94	73.402	56.055	21.163	1.00 40.38	E
MOTA	5175	NE	ARG	B	94	72.758	55.304	20.080	1.00 44.16	E

ATOM 5176 CZ ARG B 94 72.871 53.991 19.894 1.00 43.57 ATOM NH1 ARG E 94 73.602 53.259 20.720 1.00 45.04 5177 72.262 53.408 1.00 45.75 ATOM 5178 NH2 ARG R 94 18.869 R ATOM 5179 ARG E 94 77.992 57.734 22.497 1.00 29.26 77.773 ATOM 5180 0 ARG E 94 58.331 23.546 1.00 30.32 VALE 95 78.974 ATOM N 58.063 21.667 1.00 26.76 5181 ATOM 5182 CA VAL E 95 79.859 59.188 21.936 1.00 25.75 VAL B 95 81.340 58.763 21.855 1.00 22.33 ATOM 5183 СВ MOTA CG1 VAL B 95 82.244 59.914 22.287 1.00 19.80 5184 CG2 VAL E 95 ATOM 5185 81.565 57.534 22.717 1.00 19.11 Е ATOM 5186 C VAL E 95 79.600 60.266 20.902 1.00 26.51 Е VAL E 95 79.787 19.703 ATOM 5187 0 60.042 1.00 27.04 GLU B 96 79.160 61.430 21.366 1.00 27.28 ATOM 5188 N CA GLUE 96 ATOM 5189 78.870 62.536 20.466 1.00 28.16 GLU E 96 78.260 63.716 21.227 1.00 30.40 ATOM 5190 CB ATOM 5191 CG GLUE 96 76.965 63.396 21.952 1.00 34.36 CD GLU E 96 76.348 22.609 1.00 36.84 ATOM 64.625 5192 ATOM 5193 OE1 GLU E 96 75.295 64.478 23.272 1.00 38.81 OE2 GLU E 96 76.914 65.734 22.460 1.00 35.73 ATOM 5194 ATOM 5195 C GLU E 96 80.148 62.987 19.793 1.00 25.65 GLU E 96 81.176 63.171 1.00 24.93 ATOM 0 20.440 Е 5196 ATOM 5197 N PRO E 97 80.101 63.168 18.473 1.00 25.41 Е ATOM 5198 CD PRO E 97 78.977 62.979 17.539 1.00 24.36 ATOM CA PRO E 97 81.304 63.603 17.770 1.00 24.81 5199 CB PRO E 97 80.927 63.416 16.306 1.00 24.85 ATOM 5200 E ATOM 5201 CG PRO E 97 79.456 63.717 16.309 1.00 25.36 ATOM 5202 C PRO E 97 81.643 65.048 18.089 1.00 24.48 E PRO E 97 80.761 65.844 18.419 1.00 23.85 ATOM 5203 ٥ 82.927 THR E 98 18.025 1.00 22.82 ATOM 65.377 E 5204 N ATOM 5205 CA THR E 98 83.340 66.748 18.244 1.00 24.12 R THRE 98 84.679 66.852 19.019 1.00 26.31 ATOM 5206 CB MOTA OG1 THR E 98 85.744 66.355 18.205 1.00 34.47 5207 CG2 THR E 98 66.049 20.302 1.00 23.83 ATOM 5208 84.623 ATOM 5209 C THR E 98 83.519 67.254 16.817 1.00 22.12 THRE 98 84.162 15.993 1.00 21.35 ATOM 5210 0 66.601 VAL E 99 82.923 68.400 16.516 1.00 21.99 ATOM 5211 N CA VAL E 99 83.001 68.957 15.177 1.00 20.67 E ATOM 5212 1.00 19.57 ATOM 5213 CB VAL E 99 81.585 69.217 14.619 E CG1 VAL E 99 81.667 69.645 13.154 1.00 14.62 ATOM 5214 CG2 VAL E 99 C VAL E 99 80.732 67.944 14.766 1.00 15.20 ATOM 5215 70.240 15.158 1.00 22.05 ATOM 5216 83.814 ATOM 5217 0 VAL E 99 83.524 71.194 15.884 1.00 22.27 84.827 ATOM 5218 N THR E 100 70.250 14.304 1.00 21.34 E CA THR E 100 85.728 71.376 14.176 1.00 23.10 ATOM 5219 1.00 24.55 CB THR E 100 87.104 71.024 14.786 ATOM 5220 MOTA 5221 OG1 THR E 100 86.941 70.728 16.180 1.00 30.47 88.079 ATOM 5222 CG2 THR E 100 72.183 14.634 1.00 27.79 THR E 100 85.934 12.722 1.00 23.36 E ATOM 5223 С 71.777 11.842 1.00 21.77 86.024 70.926 MOTA 5224 0 THR E 100 ATOM 5225 ILE E 101 86.009 73.082 12.473 1.00 24.40 Е N ATOM 5226 CA ILE E 101 86.236 73.584 11.124 1.00 25.31 85.092 CB ILE E 101 74.518 10.645 1.00 24.21 ATOM 5227 85.398 9.245 1.00 22.51 75.044 E MOTA 5228 CG2 ILE E 101 MOTA 5229 CG1 ILE E 101 83.760 73.768 10.636 1.00 24.86 82.584 MOTA 5230 CD1 ILE E 101 74.635 10.197 1.00 25.22 ILE E 101 87.538 74.372 11.116 1.00 26.66 ATOM 5231 C 87.859 75.065 ATOM 5232 O ILE E 101 12.074 1.00 26.18 5233 **SER B 102** 88.287 74.262 10.029 1.00 31.17 MOTA N 89.547 MOTA 5234 CA SER E 102 74.977 9.902 1.00 35.36 E SER B 102 90.619 74.306 10.755 1.00 34.20 ATOM 5235 CB ATOM 5236 OG **SER E 102** 90.777 72.953 10.374 1.00 40.09 MOTA 5237 C **SER B 102** 89.976 74.979 8.448 1.00 36.82 Е 89.913 ATOM 523B 0 SER E 102 73.953 7.777 1.00 36.68 MOTA PRO E 103 90.404 76.139 7.932 1.00 39.96 5239 N 90.458 77.473 8.553 1.00 40.07 ATOM 5240 œ PRO E 103 E MOTA 5241 CA PRO E 103 90.831 76.190 6.532 1.00 42.01 PRO B 103 90.856 77.682 1.00 41.76 R ATOM 5242 CB 6.237 MOTA 5243 CG PRO E 103 91.282 78.258 7.556 1.00 42.86 MOTA 92.196 6.390 1.00 44.62 PRO E 103 75.534 5244 С ATOM 5245 0 PRO E 103 92.943 75.430 7.365 1.00 44.53 ATOM 92.514 75.086 5.181 1.00 47.92 5246 N **SER E 104** ATOM 5247 CA SER E 104 93.789 74.426 4.920 1.00 50.83 93.712 1.00 52.33 ATOM SER E 104 73.637 3.612 5248 CB 94.904 72.901 3.396 1.00 55.60 ATOM 5249 OG SER E 104

ATOM	5250	C	SER I	B 104	94.941	75.422	4.845	1.00 52.18	В
MOTA	5251	0		B 104	96.080	75.093	5.186	1.00 53.53	E
ATOM ATOM	5252	N	ASN I		90.669	78.112	-1.692	1.00 48.40	B
MOTA	5253 5254	CA CB	ASN I		90.651	77.795	-0.269	1.00 47.57	E
ATOM	5255	CG	asn i		89.863	78.854	0.496	1.00 51.34	E
ATOM	5256		L ASN E		90.504 90.693	80.219	0.417	1.00 52.99	B
ATOM	5257		2 ASN E		90.845	80.765 80.781	-0.670	1.00 55.11	E
ATOM	5258	C	ASN I		90.045	76.424	1.572 -0.001	1.00 55.09 1.00 44.87	E
ATOM	5259	0	ASN E		89.374	75.852	-0.860	1.00 44.99	e
ATOM	5260	N	LEU E	3 114	90.282	75.904	1.197	1.00 41.65	B
MOTA	5261	CA	PEA E		89.765	74.592	1.568	1.00 38.53	E
ATOM	5262	CB	LEU E		90.823	73.521	1.287	1.00 38.84	E
ATOM	5263	CG	LEU E		90.383	72.060	1.441	1.00 40.32	· E
ATOM	5264		L LEU E		89.314	71.726	0.400	1.00 39.94	E
ATOM ATOM	5265 5266		LEU E		91.586	71.145	1.266	1.00 40.52	B
ATOM	5267	0	LEU E		89.349	74.523	3.036	1.00 34.78	E
ATOM	5268	N	LEU E		90.173	74.684	3.929	1.00 33.51	E
ATOM	5269	CA	LEU E		88.063 87.550	74.293 74.181	3.278 4.641	1.00 32.05	E
ATOM	5270	CB	LEU E		86.158	74.809	4.754	1.00 29.68 1.00 29.84	E
ATOM	5271	CG	LEU E		86.046	76.257	5.241	1.00 29.84	e
MOTA	5272	CD1	LEU E	115	87.101	77.140	4.574	1.00 32.51	8
ATOM	5273	CD2	LEU E	115	84.636	76.762	4.948	1.00 30.75	E
ATOM	5274	C	LEU E		87.472	72.712	5.034	1.00 27.57	E
ATOM	5275	0	LEU E		86.871	71.900	4.331	1.00 25.33	E
ATOM	5276	N	VAL E		88.089	72.381	6.161	1.00 26.32	E
ATOM ATOM	5277	CA CB	VAL E		88.099	71.014	6.651	1.00 24.42	B
ATOM	5278 5279		VAL E VAL E		89.513	70.572	7.075	1.00 24.51	E
ATOM	5280		VALE		89.467 90.458	69.160	7.641	1.00 22.66	E
ATOM	5281	C	VAL E		87.195	70.643 70.842	5.879 7.846	1.00 26.70 1.00 22.77	E
ATOM	5282	0	VAL E		87.376	71.496	8.868	1.00 23.04	E
ATOM	5283	N	CYS E		86.208	69.968	7.717	1.00 22.34	E
ATOM	5284	CA	CYS E	117	85.326	69.711	8.840	1.00 21.65	B
ATOM	5285	C	CYS E		85.769	68.391	9.466	1.00 19.44	E
ATOM	5286	0	CYS E		85.607	67.319	8.877	1.00 18.95	E
MOTA	5287	СВ	CYS E		83.863	69.626	8.401	1.00 22.57	E
ATOM ATOM	5288 5289	SG	CYS E		82.771	69.420	9.844	1.00 25.79	E
ATOM	5299 5290	N CA	SER E		86.355	68.488	10.654	1.00 19.92	E
ATOM	5291	CB	SER E		86.837 88.115	67.330	11.387	1.00 17.98	E
ATOM	5292	OG	SER E		89.121	67.671 68.117	12.146	1.00 18.33	E
ATOM	5293	C	SER E		85.798	66.860	11.260 12.377	1.00 24.58	E
MOTA	5294	0	SER E		85.507	67.543	13.354	1.00 16.69	E
MOTA	5295	N	VAL E	119	85.240	65.688	12.112	1.00 16.58	E
MOTA	5296	CA	VAL E		84.242	65.095	12.985	1.00 16.03	B
ATOM	5297	CB			83.040	64.582	12.160	1.00 15.47	E
ATOM	5298				81.918	64.147	13.077	1.00 13.75	E
ATOM	5299		VAL E		82.559	65.686	11.216	1.00 10.95	E
MOTA MOTA	5300	C	VALE		85.018	63.960	13.638	1.00 17.51	E
ATOM	5301 5302	O N	VAL E		85.238	62.906		1.00 19.30	E
ATOM	5302	CA	THR E		85.442 86.265	64.203 63.266	14.871	1.00 18.44	E
ATOM	5304	СВ	THR E		87.562	63.962	15.616 16.042	1.00 18.41	E
ATOM	5305		THR B		87.242	65.078	16.887	1.00 18.11 1.00 17.18	e
ATOM	5306	CG2			88.304	64.481	14.835	1.00 16.77	B
ATOM	5307	C	THR E	120	85.655	62.656	16.875	1.00 20.11	E
ATOM	5308	0	THR E	120	84.665	63.148	17.417	1.00 21.96	. B
ATOM	5309	N	ASP E		86.272	61.566	17.319	1.00 19.96	E
ATOM	5310	CA	ASP E		85.882	60.B64	18.529	1.00 21.06	E
ATOM	5311	CB	ASP E		86.313	61.686	19.745	1.00 25.93	E
ATOM	5312	CG	ASP E		87.814	61.765	19.882	1.00 30.02	E
ATOM ATOM	5313 5314		ASP E		88.291	62.524	20.756	1.00 34.97	B
ATOM	5315	C	ASP E		88.513 84.431	61.063	19.114	1.00 31.15	E
ATOM	5316	0	ASP E		83.857	60.463 60.698	18.709 19.766	1.00 20.39 1.00 22.05	E
ATOM	5317	N	PHE E		83.827	59.841	17.708	1.00 22.05	e
ATOM	5318	CA	PHE E		82.443	59.429	17.873	1.00 18.28	E
MOTA	5319	СВ	PHE E	122	81.538	60.108	16.843	1.00 16.99	E
ATOM	5320	CG	PHE E	122	81.905	59.821	15.417	1.00 16.67	B
ATOM	5321		PHE E		82.770	60.661	14.725	1.00 16.72	E
MOTA	5322		PHE E		81.370	58.717	14.756	1.00 17.17	E
MOTA	5323	CEI	PHE E	122	83.096	60.410	13.384	1.00 17.00	B

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MOTA	5324		PHE I		81.686	58.456	13.419	1.00 16.82	В
ATOM	5325	CZ	PHE I		82.549	59.305	12.733	1.00 15.81	E
MOTA	5326	С	PHE 1	3 122	82.287	57.925	17.774	1.00 18.35	E
ATOM	5327	0	PHE 1	122	83.168	57.231	17.272	1.00 15.90	E
MOTA	5328	N	TYR I	3 123	81.157	57.436	18.276	1.00 19.49	E
MOTA	5329	CA	TYR I	3 123	80.818	56.021	18.243	1.00 20.92	B
ATOM	5330	CB	TYR I		81.523	55.261	19.374	1.00 21.02	E
MOTA	5331	CG	TYR I	-	81.387	53.762	19.247	1.00 20.05	E
MOTA	5332		TYR I		80.242	53.103	19.688	1.00 21.66	B
MOTA	5333		TYR I		80.095	51.726	19.516	1.00 21.85	E
ATOM	5334	CD2	TYR I	3 123	82.383	53.009	18.633	1.00 20.08	E
ATOM	5335	CE2	TYR I	3 123	82.250	51.643	18.455	1.00 19.20	E
MOTA	5336	\mathbf{cz}	TYR I	3 123	81.105	51.002	18.896	1.00 22.24	E
ATOM	5337	OH	TYR I		80.970	49.640	18.712	1.00 25.26	E
ATOM	5338	C	TYR I		79.311	55.957	18.440	1.00 21.42	B
			TYR 1						
MOTA	5339	0			78.778	56.647	19.305	1.00 23.90	E
ATOM	5340	N	PRO I		78.609	55.100	17.676	1.00 20.39	E
ATOM	5341	CD	PRO I	3 124	77.155	54.937	17.844	1.00 21.24	E
MOTA	5342	CA	PRO 1	3 124	79.113	54.177	16.655	1.00 21.61	B
MOTA	5343	CB	PRO I	3 124	77,956	53.188	16.500	1.00 19.35	B
ATOM	5344	CG	PRO 1	3 124	76.776	54.056	16.670	1.00 19.34	E
MOTA	5345	C	PRO I		79.549	54.802	15.325	1.00 20.84	E
ATOM	5346	ō	PRO I		79.602	56.024	15.184	1.00 22.13	B
									E
MOTA	5347	N		125	79.862	53.940	14.361	1.00 22.61	
MOTA	5348	CA		3 125	80.329	54.341	13.027	1.00 25.48	B
ATOM	5349	CB		3 125	80.860	53.121	12.288	1.00 26.06	E
ATOM	5350	C	ALA :	3 125	_. 79.311	55.058	12.137	1.00 27.38	E
MOTA	5351	0	ALA :	B 125	79.681	55.906	11.332	1.00 29.08	E
ATOM	5352	N	GLN :	E 126	78.039	54.706	12.268	1.00 29.18	E
ATOM	5353	CA		E 126	76.990	55.312	11.455	1.00 29.94	E
ATOM	5354	CB		E 126	75.625	54.737	11.848	1.00 33.48	E
								1.00 39.27	
ATOM	5355	CG		E 126	75.536	53.200	11.840		E
ATOM	5356	CD		E 126	76.067	52.537	13.117	1.00 41.92	E
MOTA	5357	OE1	GLN :	E 126	77.271	52.523	13.379	1.00 44.02	E
MOTA	5358	NE2	GLN :	E 126	75.159	51.981	13.913	1.00 43.83	E
ATOM	5359	C	GLN :	E 126	76.977	56.829	11.621	1.00 28.88	E
ATOM	5360	0	GLN :		76.739	57.331	12.719	1.00 28.83	B
ATOM	5361	N		E 127	77.221	57.558	10.532	1.00 27.90	E
ATOM	5362	CA		B 127	77.245	59.018	10.591	1.00 25.67	E
								1.00 25.23	E
ATOM	5363	CB	ILE		78.611	59.514	11.150		
MOTA	5364		ILE		79.693	59.398	10.084	1.00 21.16	E
MOTA	5365	CG1	ILE	E 127	78.504	60.965	11.610	1.00 22.40	E
ATOM	5366	CD1	ILE	E 127	79.610	61.376	12.546	1.00 25.35	E
MOTA	5367	С	ILE	E 127	76.985	59.673	9.230	1.00 26.38	E
ATOM	5368	0	ILE	E 127	77.196	59.065	8.182	1.00 26.20	E
ATOM	5369	N		E 128	76.521	60.916	9.252	1.00 25.64	E
		CA		B 128	76.248	61.635	8.016	1.00 29.02	E
MOTA	5370								
MOTA	5371	СВ		E 128	74.754	61.566	7.671	1.00 29.97	B
MOTA	5372	CG		B 128	74.408	62.178	6.317	1.00 35.17	E
MOTA	5373	CD		B 128	75.175	61.487	5.183	1.00 39.63	E
MOTA	5374	CE	LYS	E 128	74,936	62.163	3.836	1.00 41.20	B
ATOM	5375	NZ	LYS	B 128	75,685	61.492	2.731	1.00 44.74	E
MOTA	5376	C	LYS	E 128	76.683	63.090	8.154	1.00 28.40	E
ATOM	5377	0		B 128	76.203	63.812	9.028	1.00 27.15	E
ATOM	5378	N		B 129	77.600	63.506	7.287	1.00 28.99	В
				B 129	78.119	64.866	7.304	1.00 29.32	E
MOTA	5379	CA						1.00 30.69	
ATOM	5380	CB		E 129	79.651	64.860	7.502		E
ATOM	5381		VAL		80.171	66.282	7.654	1.00 27.54	E
MOTA	5382	CG2	VAL	B 129	80.014	64.012	8.721	1.00 30.82	E
MOTA	5383	C	VAL	E 129	77.788	65.574	5.992	1.00 30.45	e
ATOM	5384	0	VAL	B 129	78.042	65.039	4.915	1.00 30.36	E
ATOM	5385	N		E 130	77.221	66.775	6.090	1.00 31.17	E
MOTA	5386	CA		B 130	76.851	67.562	4.914	1.00 32.17	E
				E 130				1.00 34.73	E
ATOM	5387	СВ			75.330	67.626	4.764		
MOTA	5388	CG		E 130	74.632	66.335	4.400	1.00 40.85	E
MOTA	5389	СD		E 130	73.121	66.527	4.511	1.00 46.16	E
MOTA	5390	NE		E 130	72.365	65.456	3.864	1.00 51.33	E
MOTA	5391	CZ	ARG	E 130	71.046	65.308	3.959	1.00 53.45	E
MOTA	5392		ARG	E 130	70.327	66.162	4.680	1.00 54.21	E
ATOM	5393			E 130	70.444	64.307	3.329	1.00 53.97	E
ATOM	5394	C		E 130	77.359	68.994	5.017	1.00 30.88	B
		Ö		B 130	77.321	69.590	6.093	1.00 30.84	B
MOTA	5395							1.00 29.14	E
MOTA	5396	N		B 131	77.831	69.542	3.900		
MOTA	5397	CA	TRP	E 131	78.291	70.928	3.865	1.00 29.57	B

ATOM 5398 CB TRP E 131 79.538 71.086 2.996 1.00 27.97 ATOM 5399 CG TRP E 131 80.809 70.979 3.760 1.00 29.37 MOTA Е 5400 CD2 TRP E 131 81.342 71.949 4.671 1.00 29.95 В ATOM 5401 CE2 TRP B 131 82.551 71.427 5.174 1.00 29.75 ATOM 5402 CE3 TRP E 131 80.913 73.209 1.00 30.39 5.111 R ATOM 5403 CD1 TRP E 131 81.689 69.941 3.747 1.00 29.02 ATOM 5404 NE1 TRP E 131 82.738 70.200 4.592 1.00 30.01 ATOM 5405 CZ2 TRP E 131 83.340 72.119 6.095 1.00 28.79 ATOM 5406 CZ3 TRP E 131 81.697 73.900 6.027 1.00 31.30 ATOM 5407 CH2 TRP E 131 82.900 73.350 6.509 1.00 31.69 ATOM 5408 С TRP E 131 77.185 71.817 3.301 1.00 30.08 ATOM TRP E 131 5409 0 76.449 71.413 2.392 1.00 29.15 ATOM 5410 N PHE E 132 77.081 73.027 3.842 1.00 29.87 E ATOM 5411 CA PHE E 132 76.078 73.985 3.405 1.00 30.98 E ATOM 5412 CB PHE E 132 74.963 74.094 4.443 1.00 32.09 ATOM CG PHE E 132 5413 74.041 72.918 4.461 1.00 33.03 E ATOM 5414 CD1 PHE E 132 72.913 72.896 3.650 1.00 35.25 ATOM 5415 CD2 PHE E 132 74.306 71.822 5.273 1.00 33.31 R ATOM 5416 CE1 PHE E 132 72.055 71.794 3.646 1.00 35.49 ATOM 5417 CE2 PHE E 132 73.460 70.717 5.279 1.00 35.47 ATOM 5418 CZ PHE E 132 72.330 70.704 4.461 1.00 35.97 B ATOM PHE B 132 5419 C 76.668 75.364 3.182 1.00 32.06 ATOM 5420 PHE E 132 77.537 75.812 3.929 1.00 29.15 ATOM 5421 N ARG E 133 76.186 76.026 2.138 1.00 34.68 ATOM 5422 CA ARG E 133 76.613 77.375 1.809 1.00 37.78 ATOM 5423 CB ARG E 133 77.281 77.420 0.434 1.00 40.14 \mathbf{E} ATOM 5424 CG ARG E 133 77.755 78.810 0.005 1.00 43.27 B ATOM 5425 Ф ARG E 133 78.474 78.742 -1.341 1.00 46.34 ATOM 5426 NB ARG E 133 79.096 80.006 -1.738 1.00 49.86 ATOM ARG E 133 5427 cz78.441 81.058 -2.226 1.00 51.63 ATOM 5428 NH1 ARG E 133 77.124 81.018 -2.387 1.00 51.33 ATOM 5429 NH2 ARG E 133 79.111 82.155 -2.562 1.00 52.46 ATOM 5430 C ARG E 133 75.343 78.204 1.792 1.00 38.70 ATOM 5431 0 ARG E 133 74.569 78.154 0.835 1.00 38.81 ATOM 5432 N **ASN B 134** 75.119 78.940 2.872 1.00 39.37 E ATOM 5433 CA ASN E 134 73.941 79.787 2.984 1.00 42.21 ATOM 5434 CB ASN E 134 74.040 80.952 1.988 1.00 40.37 B ATOM 5435 CG ASN E 134 75.383 81.667 2.051 1.00 39.50 R ATOM 5436 OD1 ASN E 134 75.796 82.151 3.104 1.00 35.36 ATOM 5437 ND2 ASN E 134 76.071 81.733 0.917 1.00 39.94 ATOM 5438 C **ASN E 134** 72.652 79.000 2.734 1.00 43.61 B ATOM 5439 O ASN E 134 71.899 79.306 1.809 1.00 45.62 R ATOM 5440 N ASP E 135 72.403 77.983 3.550 1.00 45.40 E ATOM 5441 CA ASP E 135 71.189 77.178 3.413 1.00 47.16 ATOM 5442 C **ASP E 135** 71.147 76.279 2.173 1.00 48.15 R ASP E 135 MOTA 5443 O 70.205 75.504 1.996 1.00 49.25 R MOTA GLN E 136 5444 N 72.158 76.387 1.316 1.00 48.16 5445 CA MOTA GLN E 136 72.226 75.561 0.113 1.00 47.50 ATOM 5446 C **GLN E 136** 73.254 74.445 0.313 1.00 47.38 ATOM 5447 0 GLN E 136 74.418 74.711 0.627 1.00 46.25 B ATOM 5448 N **GLU E 137** 72.829 73.197 0.139 1.00 47.09 MOTA 5449 CA **GLU E 137** 73.749 72.079 0.308 1.00 47.41 ATOM 5450 CB GLU B 137 72.992 70.752 0.406 1.00 47.53 R ATOM **GLU E 137** 5451 CG 73.921 69.570 0.653 1.00 49.67 MOTA 5452 CD GLU E 137 73.210 68.334 1.166 1.00 51.28 ATOM 5453 OE1 GLU E 137 73.911 67.336 1.432 1.00 52.31 ATOM 5454 OE2 GLU E 137 71.965 68.352 1.306 1.00 51.54 ATOM 5455 C **GLU E 137** 74.755 72.016 -0.833 1.00 47.37 R ATOM 5456 ٥ **GLU E 137** 74.397 72.163 -2.000 1.00 47.51 Ε ATOM 5457 N **GLU E 138** 76.018 71.809 -0.477 1.00 47.53 MOTA 5458 CA **GLU E 138** 77.104 71.724 -1.444 1.00 48.48 ATOM 5459 CB **GLU E 138** 78.266 -1.011 1.00 49.89 72.617 ATOM 5460 CG **GLU E 138** 77.949 74.096 -0.973 1.00 54.83 ATOM 5461 CD **GLU B 138** 77.911 74.720 -2.354 1.00 57.91 ATOM 5462 OE1 GLU E 138 78.953 74.686 1.00 59.04 -3.044 MOTA 5463 OE2 GLU E 138 76.846 75.247 1.00 58.96 -2.748 ATOM 5464 С **GLU E 138** 77.593 -1.532 1.00 48.42 70.284 MOTA 5465 GLU E 138 0 77.898 69,665 -0.513 1.00 48.62 ATOM 5466 THR E 139 N 77.665 69.754 -2.748 1.00 47.87 ATOM 5467 CA THR E 139 78.135 68.387 1.00 48.16 -2.959 ATOM 5468 CB THR E 139 77.027 67.498 -3.556 1.00 49.05 ATOM 5469 OG1 THR E 139 76.464 68.140 1.00 51.25 -4.710 R 5470 CG2 THR E 139 75.938 67.249 -2.525 1.00 48.03 MOTA 5471 C THR E 139 79.339 68.401 -3.895 1.00 46.96

ATOM	5472	0		B 139	80.245	67.574	-3.779	1.00 46.46	E
MOTA	5473	N		E 140	79.339	69.346	-4.827	1.00 46.59	E
MOTA MOTA	5474	CA		B 140	80.446	69.488	-5.761	1.00 45.07	E
ATOM	5475 5476	CB C		E 140 E 140	79.997	70.244	-7.008	1.00 44.64	E
ATOM	5477	ŏ		E 140	81.518 81.224	70.276	-5.019	1.00 43.57	E
ATOM	5478	N		B 141	82.756	71.293 69.805	-4.386 -5.091	1.00 43.33	E
ATOM	5479	CA		E 141	83.833	70.485	-4.398	1.00 41.31 1.00 38.27	E
ATOM	5480	C		B 141	84.053	69.854	-3.034	1.00 36.91	e E
ATOM	5481	0	GLY	E 141	84.930	70.264	-2.272	1.00 37.78	B
ATOM	5482	N		B 142	83.245	68.849	-2.722	1.00 33.36	E
ATOM	5483	CA		B 142	83.363	68.164	-1.449	1.00 32.16	E
ATOM ATOM	5484	CB		B 142	81.978	67.844	-0.847	1.00 31.40	E
ATOM	5485 5486		VAL		82.140	66.995	0.407	1.00 28.96	E
ATOM	5487	C		B 142	81.245 84.140	69.134 66.859	-0.516	1.00 33.20	E
ATOM	5488	ŏ		E 142	83.862	66.032	-1.576 -2.450	1.00 31.49	E
ATOM	5489	N		B 143	85.118	66.684	-0.696	1.00 31.67 1.00 30.51	E
MOTA	5490	CA		E 143	85.922	65.473	-0.675	1.00 30.35	E
MOTA	5491	CB	VAL :	E 143	87.367	65.731	-1.161	1.00 30.33	E
ATOM	5492		VAL I		88.096	64.408	-1.348	1.00 32.44	_ B
ATOM	5493		VAL		87.347	66.503	-2.460	1.00 33.96	B
ATOM	5494	C		B 143	85.966	64.973	0.767	1.00 29.68	E
ATOM ATOM	5495	0		143	86.242	65.733	1.695	1.00 29.63	E
ATOM	5496 5497	N CA		B 144 B 144	85.696	63.689	0.946	1.00 28.32	E
ATOM	5498	СВ		E 144	85.703 84.295	63.090 62.613	2.268	1.00 25.38	E
ATOM	5499	OG		3 144	84.300	61.845	2.622 3.807	1.00 26.70 1.00 28.37	E
ATOM	5500	C		E 144	86.663	61.916	2.361	1.00 24.56	e
ATOM	5501	0	SER 1	8 144	86.824	61.148	1.412	1.00 23.42	E
ATOM	5502	N		3 145	87.320	61.790	3.506	1.00 24.40	B
ATOM	5503	CA		3 145	88.218	60.666	3.726	1.00 24.38	E
ATOM	5504	CB		3 145	89.103	60.849	4.983	1.00 24.55	E
ATOM ATOM	5505		THR I		88.273	60.815	6.155	1.00 21.59	R
ATOM	5506 5507	C	THR I		89.858	62.162	4.935	1.00 24.64	B
ATOM	5508	Ö	THR I		87.256 86.064	59.539	4.055	1.00 23.78	E
ATOM	5509	N	PRO I		87.745	59.766 58.300	4.242 4.099	1.00 23.97	E
ATOM	5510	CD	PRO E		88.993	57.713	3.585	1.00 25.25 1.00 25.42	e
MOTA	5511	CA	PRO E		86.770	57.264	4.447	1.00 25.00	E
MOTA	5512	CB	PRO E	146	87.439	55.983	3.951	1.00 26.60	E
ATOM	5513	CĠ	PRO E		88.905	56.293	4.094	1.00 27.24	E
ATOM	5514	C	PRO E		86.597	57.284	5.976	1.00 23.26	E
ATOM	5515	0	PRO E		87.286	58.030	6.672	1.00 21.73	B
ATOM ATOM	5516 5517	n Ca	LEU E		85.669	56.492	6.495	1.00 23.85	E
ATOM	5518	CB	LEU E		85.476	56.419	7.936	1.00 23.63	B
ATOM	5519	CG	LEU E		84.355 83.976	55.428 55.241	8.260 9.731	1.00 25.11	E
ATOM	5520		LEU B		83.392	56.530	10.270	1.00 28.28 1.00 29.44	e
ATOM	5521		LEU E		82.965	54.116	9.867	1.00 28.72	E
MOTA	5522	C	LEU E		86.812	55.915	8.503	1.00 22.77	B
MOTA	5523	0	TEA E	147	87.366	54.944	8.003	1.00 23.04	E
MOTA	5524	N	ILE E		87.337	56.574	9.530	1.00 21.06	E
MOTA	5525	CA	ILE E		88.614	56.156	10.102	1.00 19.40	E
ATOM ATOM	5526	CB	ILE E		89.588	57.355	10.200	1.00 20.05	E
ATOM	5527 5528		ILE E		90.903	56.922	10.835	1.00 19.93	E
ATOM	5529		ILE E		89.854 90.594	57.918 59.225	8.803 8.821	1.00 17.58	B
ATOM	5530	c	ILE E		88.449	55.534	11.489	1.00 20.23 1.00 17.19	В
ATOM	5531	0	ILE E		87.820	56.118	12.360	1.00 17.19	e
ATOM	5532	N	ARG E		89.015	54.344	11.677	1.00 15.23	E
ATOM	5533	CA	ARG E	149	88.948	53.638	12.956	1.00 16.42	E
ATOM	5534	CB	ARG E		88.906	52.128	12.724	1.00 20.12	E
ATOM	5535	CG	ARG E		88.903	51.289	14.000	1.00 21.32	E
ATOM ATOM	5536 5537	NE CD	ARG E		88.963	49.802	13.649	1.00 22.44	B
ATOM ATOM	5537	CZ	ARG E		87.825	49.382	12.830	1.00 22.55	E
ATOM	5539		ARG E		86.623 85.650	49.084 48.718	13.313 12.490	1.00 22.89	E
ATOM	5540		ARG E		86.398	49.139	14.619	1.00 24.25 1.00 23.36	e B
ATOM	5541	С	ARG E		90.174	53.983	13.786	1.00 16.33	B
MOTA	5542	0	ARG E	149	91.305	53.734	13.363	1.00 16.45	В
MOTA	5543	N	asn e		89.953	54.558	14.963	1.00 15.72	B
MOTA	5544	CA	ASN B		91.061	54.948	15.825	1.00 15.93	E
MOTA	5545	CB	asn e	150	90.662	56.125	16.740	1.00 13.37	E
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MOTA	5546	CG	aen e	3 :	150	90.278	57.383	15.955	1.00	15.55	E
MOTA	5547		asn i			90.922	57.739	14.955		14.20	E
MOTA	5548		ASN E			89.233	58.068	16.414		15.61	E
MOTA	5549	C	ASN I			91.576	53.786	16.670		16.79	E
ATOM ATOM	5550 5551	o N	ASN E			92.694 90.764	53.838 52.745	17.180 16.813		18.80 16.63	E
MOTA	5552	CA	GLY I			91.164	51.587	17.593		18.68	E
ATOM	5553	C	GLY I			90.879	51.684	19.080		20.19	E
ATOM	5554	ō	GLY I			91.087	50.725	19.818		21.39	B
MOTA	5555	N	ASP I			90.409	52.836	19.539		19.57	E
MOTA	5556	CA	ASP I	3	152	90.108	52.986	20.954	1.00	19.09	E
ATOM	5557	CB	ASP I			90.865	54.177	21.531	1.00	18.53	E
MOTA	5558	CG	ASP I			90.498	55.481	20.856		21.27	E
ATOM	5559		ASP I			89.736	55.453	19.864	-	20.11	E
MOTA	5560		ASP I			90.984	56.531	21.321		22.57 19.23	e
ATOM ATOM	5561 5562	С 0	ASP I			88.605 88.177	53.156 53.840	21.182 22.113		17.78	13
ATOM	5563	N	TRP 1			87.816	52.522	20.318		18.88	E
ATOM	5564	CA	TRP 1			86.356	52.566	20.391		18.61	B
ATOM	5565	CB	TRP 1			85.862	52.162	21.788	1.00	17.06	B
MOTA	5566	CG	TRP I	3	153	86.084	50.690	22.085	1.00	17.90	B
MOTA	5567	CD2	TRP		153	85.165	49.612	21.830		18.84	R
ATOM	5568		TRP :			85.804	48.414	22.222		16.88	B
MOTA	5569		TRP			83.862	49.544	21.308		18.29	B
MOTA	5570		TRP			87.209	50.114	22.604		16.70 17.49	e
ATOM	5571	NEI	TRP I			87.049 85.189	48.747 47.164	22.688 22.109		16.54	E
MOTA MOTA	5572 5573	CZ3	TRP			83.250	48.303	21.196		17.19	E
ATOM	5574	CH2	TRP			83.917	47.129	21.597		17.24	E
ATOM	5575	C	TRP			85.732	53.887	19.975		18.97	E
ATOM	5576	ō	TRP			84.696	54.300	20.508	1.00	18.70	В
MOTA	55 7 7	N	THR :	В	154	86.378	54.546	19.016	1.00	19,20	E
MOTA	5578	CA	THR	B	154	85.876	55.794	18.444	1.00	19.92	E
ATOM	5579	CB	THR			86.442	57.072	19.129		21.42	E
MOTA	5580		THR			87.865	57.129	18.958		19.26	E
ATOM	5581		THR			86.085	57.096	20.599		22.17	E
ATOM	5582	C	THR			86.314	55.835	16.992		18.66 19.45	E
MOTA	5583	0	THR			87.270 85.609	55.156 56.626	16.603 16.193		18.54	2
ATOM ATOM	5584 5585	N CA			155	85.940	56.784	14.779		19.04	E
MOTA	5586	СВ	PHE			84.821	56.252	13.882		20.71	E
ATOM	5587	CG	PHE			84.524	54.794	14.060		23.03	B
ATOM	5588		PHE	E	155	83.492	54.375	14.898	1.00	23.94	E
ATOM	5589	CD2	PHE	E	155	85.255	53.837	13.365	1.00	23.32	B
MOTA	5590		PHE			83.189	53.017	15.037		23.82	B
ATOM	5591	CE2				84.962	52.476	13.497		24.46	B
MOTA	5592	CZ	PHE			83.930	52.068	14.333		24.51 19.30	e B
ATOM	5593	C	PHE			86.109 85.791	58.265 59.134	14.459 15.275		19.30	E
MOTA MOTA	5594 5595	N	GLN			86.613	58.550	13.265		17.46	B
ATOM	5596	CA	GLN			86.748	59.924	12.824		17.87	E
ATOM	5597	CB	GLN			88.081	60.546	13.264		19.74	В
MOTA	5598	CG	GLN	B	156	89.330	59.948	12.640	1.00	19.80	E
MOTA	5599	CD	GLN	E	156	90.551	60.785	12.950		21.46	B
MOTA	5600		GLN			90.660	61.928	12.503		21.30	E
MOTA	5601		GLN			91.469	60.230	13.734		21.38	E
MOTA	5602	C	GLN			86.629	59.989	11.316 10.616		17.47 17.25	B E
MOTA	5603 5604	И	GLN ILE			86.856 86.252	58.999 61.159	10.823		17.46	E
MOTA MOTA	5605	CA	ILE			86.128	61.363	9.397		18.92	E
ATOM	5606	CB	ILE			84.746	60.922	8.898		19.57	E
ATOM	5607		ILE			83.659	61.774	9.545		15.09	E
MOTA	5608		ILE			84.704	60.994	7.369	1,00	21.06	B
ATOM	5609		ILE			83.541	60.218	6.756		22.57	E
ATOM	5610	C	ILE			86.349	62.837	9.083		20.28	B
MOTA	5611	0	ILE			85.887	63.712	9.808		20.70	B
ATOM	5612	N	LEU			87.094	63.104	8.019		21.79	E
MOTA	5613	CA	LEU			87.363	64.470	7.601 7.466		23.40	e E
MOTA	5614 5615	CB CG	LEU		158 158	88.869 89.621	64.706 65.141	8.731		29.38	E
MOTA MOTA	5616		LEU			89.384	64.154	9.864		27.98	E
ATOM	5617		2 LEU			91.118	65.263	8.412		30.79	B
ATOM	5618	c			158	86.664	64.738	6.271		23.62	E
MOTA	5619	0			158	86.938	64.081	5.264	1.00	22.86	E

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ATOM	5620	N	VAL E 159	85.747	65.702	6.290	1.00 22.98	B
MOTA	5621	CA	VAL E 159	84.990	66.087	5.112	1.00 21.37	E
ATOM	5622	CB	VAL E 159	83.476	66.104	5.417	1.00 20.53	E
MOTA	5623	CG1	VAL E 159	82.684	66.407	4.149	1.00 14.20	E
ATOM	5624		VAL E 159	83.058	64.756	6.002	1.00 15.86	B
			VAL E 159	85.468	67,469	4.710	1.00 22.21	E
ATOM	5625	C					1.00 22.87	E
MOTA	5626	0	VAL B 159	85.253	68.444	5.423		
MOTA	5627	N	MET E 160	86.116	67.539	3.555	1.00 25.37	E
ATOM	5628	CA	MET B 160	86.681	68.779	3.049	1.00 27.07	E
MOTA	5629	СВ	MET B 160	88.088	68.494	2.533	1.00 29.57	E
ATOM	5630	CG	MET E 160	88.996	67.954	3.633	1.00 35.17	E
					67.185	3.065	1.00 41.54	E
MOTA	5631	SD	MET E 160	90.519				B
MOTA	5632	CE	MET E 160	90.011	65.462	2.985	1.00 40.10	
ATOM	5633	C	MET R 160	85.848	69.466		1.00 28.93	E
ATOM	5634	0	MET E 160	85.191	68.817	1.162	1.00 28.47	B
MOTA	5635	N	LEU E 161	85.875	70.793	1.997	1.00 29.41	E
ATOM	5636	CA	LEU E 161	85.123	71.574	1.031	1.00 31.54	B
			LEU B 161	83.931	72.258	1.708	1.00 30.26	E
ATOM	5637	СВ						E
ATOM	5638	CG	LEU E 161	83.183	73.297	0.860	1.00 30.70	
MOTA	5639	CD1	LEU E 161	82.515	72.618	-0.332	1.00 29.72	E
ATOM	5640	CD2	LEU B 161	82.145	74.020	1.728	1.00 31.55	E
ATOM	5641	C	LEU E 161	85.990	72.625	0.363	1.00 32.10	B
ATOM	5642	ō	LEU E 161	86.575	73.473	1.029	1.00 32.90	E
			GLU E 162		72.549	-0.960	1.00 35.11	B
MOTA	5643	N		86.063				E
ATOM	5644	CA	GLU E 162	86.820	73.491	-1.771	1.00 38.40	
ATOM	5645	CB	GLU E 162	87.191	72.838	-3.105	1.00 42.17	B
MOTA	5646	CG	GLU E 162	87.783	73.776	-4.148	1.00 48.21	B
ATOM	5647	CD	GLU E 162	89.099	74.381	-3.711	1.00 52.47	E
ATOM	5648		GLU E 162	90.006	73.611	-3.327	1.00 54.02	B
						-3.759	1.00 56.21	B
MOTA	5649		GLU E 162	89.228	75.627			
MOTA	5650	C	GLU E 162	85.892	74.673	-2.008	1.00 39.06	E
MOTA	5651	0	GLU E 162	84.750	74.490	-2.422	1.00 39.27	E
MOTA	5652	N	MET E 163	86.369	75.884	-1.747	1.00 40.73	E
MOTA	5653	CA	MET E 163	85.520	77.049	-1.938	1.00 43.18	B
		CB	MET B 163	84.546	77.171	-0.761	1.00 45.15	B
MOTA	5654						1.00 47.55	E
ATOM	5655	CG	MET E 163	85.155	76.900	0.612		
MOTA	5656	SD	MET E 163	86.318	78.152	1.185	1.00 52.18	B
MOTA	5657	CE	MET B 163	85.186	79.345	1.941	1.00 50.37	E
ATOM	5658	C	MET E 163	86.245	78.371	-2.151	1.00 43.77	E
ATOM	5659	ō	MET E 163	87.458	78.477	-1.953	1.00 41.87	E
			THR E 164	85.474	79.371	-2.571	1.00 45.83	E
MOTA	5660	N					1.00 49.20	E
MOTA	5661	CA	THR E 164	85.981	80.714	-2.827		
MOTA	5662	CB	THR E 164	85.585	81.177	-4.241	1.00 50.11	E
MOTA	5663	OG1	THR E 164	86.036	80.208	-5.199	1.00 49.28	E
ATOM	5664	CG2	THR E 164	86.204	82.535	-4.559	1.00 50.19	B
ATOM	5665	С	THR E 164	85.371	81.652	-1.785	1.00 51.14	E
ATOM	5666	ō	THR B 164	84.169	81.916	-1.802	1.00 50.64	E
			PRO E 165	86.198	82.170	-0.864	1.00 53.75	B
MOTA	5667	N					1.00 54.65	E
MOTA	5668	CD	PRO B 165	87.667	82.057	-0.818		
MOTA	5669	CA	PRO E 165	85.719	83.072	0.185	1.00 56.16	E
ATOM	5670	CB	PRO E 165	86.965	83.299	1.036	1.00 55.47	B
ATOM	5671	ÇG	PRO E 165	88.057	83.262	0.019	1.00 55.93	E
ATOM	5672	C	PRO B 165	85.098	84.381	-0.291	1.00 58.83	E
ATOM		ŏ	PRO E 165	85.673	85.100	-1.112	1.00 58.35	E
	5673				84.666	0.239	1.00 61.77	B
ATOM	5674	N	GLN B 166	83.912				E
ATOM	5675	CA	GLN E 166	83.173	85.885	-0.065	1.00 63.96	
MOTA	5676	CB	GLN E 166	82.103	85.616	-1.123	1.00 64.28	E
MOTA	5677	CG	GLN E 166	82.662	85.236	-2.481	1.00 66.42	B
ATOM	5678	CD	GLN E 166	81.643	85.392	-3.596	1.00 67.38	E
MOTA	5679		L GLN E 166	81.937	85,124	-4.761	1.00 68.28	; E
			2 GLN B 166	80.437	85.832	-3.244	1.00 66.50	E
MOTA	5680					1.223	1.00 65.40	B
MOTA	5681	С	GLN E 166	82.521	86.396			
MOTA	5682	0	GLN E 166	81.974	85.614	2.007	1.00 65.65	E
ATOM	5683	N	ARG E 167	82.589	87.707	1.444	1.00 65.80	E
ATOM	5684	CA	ARG E 167	82.017	88.302	2.647	1.00 65.27	B
MOTA	5685	CB	ARG E 167	82.353	89.795	2.706	1.00 67.87	E
		CG		82.221		4.095	1.00 70.91	E
ATOM	5686					5.085	1.00 73.36	B
ATOM	5687		ARG E 167	83.216				E
MOTA	5688			83.244		6.359	1.00 75.19	
MOTA	5689	CZ		84.012		7.394	1.00 75.48	E
MOTA	5690	NH	1 ARG B 167	84.824	89.151	7.318	1.00 75.50	E
MOTA	5691		2 ARG E 167	83.968	90.916	8.509	1.00 75.83	E
ATOM	5692		ARG E 167	80.504	_	2.684	1.00 63.81	E
ATOM			ARG E 167	79.816		1.672		E
AL ON	5693	9	10 to 10 t	,,,,,,	-0.234	_,,,,	~	

ATOM	5694	N	GLY E	168	79.991	87.751	3.860	1.00 61.88	E
MOTA	5695	CA	GLY E	168	78.567	87.519	4.004	1.00 58.78	E
ATOM	5696	C	GLY E		78.243	86.036	3.959	1.00 57.24	E
								1.00 57.26	Б
MOTA	5697	0	GLY E		77.262	85.594	4.558		
MOTA	5698	N	ASP E		79.066	85.263	3.249	1.00 54.67	E
MOTA	5699	CA	ASP E	169	78.849	83.823	3.140	1.00 52.07	E
MOTA	5700	CB	ASP E	169	79.799	83.186	2.116	1.00 52.03	E
ATOM	5701	CG	ASP E		79.329	83.359	0.683	1.00 52.57	E
	5702		ASP E		78.105	83.453	0.457	1.00 51.86	R
ATOM									
MOTA	5703		ASP E		80.188	83.376	-0.223	1.00 52.34	B
ATOM	5704	C	ASP B	169	79.027	83.096	4.463	1.00 49.54	E
MOTA	5705	0	ASP E	169	79.993	83.322	5.196	1.00 49.84	B
MOTA	5706	N	VAL E	170	78.082	82.214	4.758	1.00 46.54	E
MOTA	5707	CA	VAL E		78.136	81.418	5.970	1.00 43.15	B
							6.871		
MOTA	5708	CB	VAL E		76.903	81.669		1.00 42.70	E
MOTA	5709		VAL E		76.997	80.819	8.138	1.00 41.36	B
ATOM	5710	CG2	VAL B	170	76.814	83.146	7.227	1.00 41.14	E
ATOM	5711	С	VAL E	170	78.172	79.948	5.555	1.00 41.66	B
MOTA	5712	0	VAL E	170	77.216	79.432	4.972	1.00 40.25	E
ATOM	5713	N	TYR E		79.289	79.287	5.833	1.00 39.16	E
							5.502	1.00 38.16	E
ATOM	5714	CA	TYR E		79.438	77.877			
MOTA	5715	CB	TYR E		80.836	77.617	4.953	1.00 38.66	E
MOTA	5716	CG	TYR E	171	81.035	78.237	3.598	1.00 38.98	B
ATOM	5717	CD1	TYR E	171	80.740	77.522	2.440	1.00 38.79	B
ATOM	5718	CK1	TYR E	171	80.852	78.105	1.186	1.00 40.42	E
ATOM	5719		TYR E		81,451	79.561	3.471	1.00 38.62	B
								1.00 40.32	E
ATOM	5720		TYR E		81.565	80.160	2.219		
ATOM	5721	CZ	TYR E	171	81.262	79.424	1.079	1.00 41.26	B
MOTA	5722	OH	TYR E	171	81.350	80.004	-0.166	1.00 42.98	B
MOTA	5723	С	TYR E	171	79.206	77.076	6.764	1.00 37.15	B
ATOM	5724	Ō	TYR E		79.755	77.398	7.813	1.00 37.94	E
		N	THR E		78.384	76.037	6.672	1.00 35.12	E
MOTA	5725					75.229		•	E
MOTA	5726	CA	THR E		78.091		7.842	1.00 34.42	
ATOM	5727	CB	THR E		76.654	75.496	8.367	1.00 35.21	E
MOTA	5728	OG1	THR E	172	76.184	74.351	9.094	1.00 35.96	E
MOTA	5729	CG2	THR E	172	75.706	75.790	7.226	1.00 38.35	E
MOTA	5730	С	THR E		78.263	73.734	7.638	1.00 32.90	B
			THR E		77.875	73.188	6.604	1.00 31.57	E
MOTA	5731	0							B
MOTA	5732	N	CYS E		78.858	73.090	8.643	1.00 30.59	
ATOM	5733	CA	CYS E	173	79.078	71.646	8.640	1.00 29.35	E
MOTA	5734	С	CYS E	173	77.923	71.058	9.454	1.00 29.72	E
ATOM	5735	0	CYS E	173	77.771	71.337	10.645	1.00 28.89	E
ATOM	5736	CB	CYS E	173	80.424	71.299	9.287	1.00 27.53	E
		SG	CYS E		80.875	69.541	9.133	1.00 27.81	E
MOTA	5737							1.00 28.95	E
MOTA	5738	N	HIS E		77.109	70.251	8.788		
MOTA	5739	CA	HIS E	174	75.925	69.642	9.381	1.00 28.54	E
ATOM	5740	CB	HIS E	174	74.770	69.881	8.399	1.00 29.66	B
ATOM	5741	CG	HIS E	174	73.457	69.311	8.823	1.00 30.98	E
ATOM	5742	CD2	HIS E	174	72.367	69.899	9.369	1.00 31.91	E
ATOM	5743		HIS E		73.124	67.988	8.630	1.00 31.68	E
			HIS E			67.785	9.034	1.00 33.26	B
ATOM	5744				71.883				E
ATOM	5745		HIS E		71.401	68.929	9.487	1.00 34.66	
ATOM	5746	C	HIS E	3 174	76.173	68.151	9.650	1.00 27.83	E
ATOM	5747	0	HIS E	E 174	76.438	67.375	8.728	1.00 27.35	B
ATOM	5748	N	VAL E	3 175	76.085	67.753	10.917	1.00 26.27	E
ATOM	5749	CA	VAL E		76.349	66.365	11.284	1.00 26.34	B
ATOM	5750	СВ	VAL I		77.584	66.281	12.215	1.00 23.90	E
					77.807			1.00 19.67	B
ATOM	5751		. VAL I			64.850	12.663		
MOTA	5752		VAL I		78.818	66.813	11.491	1.00 19.93	B
MOTA	5753	C	VAL I	3 175	75.199	65.603	11.938	1.00 27.67	E
MOTA	5754	0	VAL I	3 175	74.587	66.064	12.904	1.00 26.77	E
MOTA	5755	N	GLU I	3 176	74.917	64.423	11.399	1.00 29.83	B
MOTA	5756	CA		3 176	73.864	63.564	11.929	1.00 32.99	E
					72.842	63.231	10.839	1.00 34.86	E
ATOM	5757	CB		3 176					E
ATOM	5758	CG		E 176	72.076	64.441	10.319	1.00 40.13	
MOTA	5759	æ	GTD 1	E 176	71.204	64.107	9.124	1.00 44.38	E
MOTA	5760	OE:	L GLU	E 176	70.292	63.265	9.269	1.00 46.31	B
ATOM	5761	OE:		E 176	71.433	64.682	8.037	1.00 47.49	E
MOTA	5762	C		E 176	74.526	62.289	12.445	1.00 32.24	E
					75.296	61.646	11.734	1.00 32.81	E
MOTA	5763	0		E 176				1.00 32.61	E
ATOM	5764	N		E 177	74.220	61.934	13.686		B
MOTA	5765	CA		B 177	74.803	60.761	14.311	1.00 30.50	
ATOM	5766	CB	HIS !	E 177	76.147	61,161	14.927	1.00 29.59	E
ATOM	5767	CG	HIS:	E 177	76.871	60.034	15.582	1.00 28.23	E

MOTA	5768	സാ	HIS	R	177	77.752	59.134	15.086	3 00	28.22	73
											E
ATOM	5769		HIS			76.679	59.698	16.903		27.71	B
MOTA	5770		HIS			77.410	58.636	17.194		29.83	B
MOTA	5771		HIS			78.070	58.274	16.108	1.00	29.78	B
MOTA	5772	C	HIS	E	177	73.854	60.195	15.373	1.00	30.09	E
MOTA	5773	0	HIS	ĸ	177	73.189	60.942	16.083	1.00	29.91	B
MOTA	5774	N	PRO	E	176	73.781	58.862	15.496	1.00	31.45	B
MOTA	5775	CD	PRO			74.485	57.842	14.697		31.00	B
ATOM	5776	CA	PRO			72.898	58.226	16.481		31.44	B
MOTA	5777	CB	PRO		178	73.370	56.779	16.467		30.89	E
ATOM	5778	CG	PRO			73.704	56.578	15.028		31.16	E
MOTA	5779	C	PRO	E	178	72.896	58.826	17.893	1.00	31.78	B
MOTA	5780	0	PRO	B	178	71.903	58.727	18.611	1.00	32.84	B
ATOM	5781	N	SER	E	179	73.996	59.448	18.292	1.00	30.31	B
ATOM	5782	CA	SER			74.087	60.039	19.624		30.84	B
MOTA		CB	SER				60.155			29.11	R
	5783					75.552		20.038			
MOTA	5784	OG	SER			76.240	61.049	19.176		24.79	B
MOTA	5785	С	SER			73.452	61.424	19.717		32.75	B
MOTA	5786	0	SER	B	179	73.330	61.982	20.804	1.00	32.78	B
ATOM	5787	N	LEU	B	180	73.046	61.981	18.583	1.00	35.18	E
ATOM	5788	CA	LEU	В	180	72.477	63.317	18.578	1.00	37.31	E
MOTA	5789	CB	LEU			73.098	64.132	17.448		35.77	E
ATOM	5790	CG	LEU			74.610	64.337	17.528		36.46	E
											E
ATOM	5791		TEO			75.097	65.018	16.259		35.16	
MOTA	5792		LEU			74.948	65.167	18.752		34.58	E
MOTA	5793	С	LEU	E	180	70.967	63.405	18.463	1.00	40.35	E
MOTA	5794	0	LEU	E	180	70.386	63.003	17.456	1.00	40.67	E
MOTA	5795	N	GLN	B	181	70.338	63.943	19.503	1.00	42.97	E
ATOM	5796	CA	GLN			68.895	64.141	19.504		45.09	E
ATOM	5797	CB	GLN			68.466	64.877	20.776		46.73	E
							65.931				E
MOTA	5798	CG	GLN			69.471		21.235		49.84	
MOTA	5799	CD	GFN			68.898	66.904	22.256		52.17	E
ATOM	5800	ob1	\mathbf{GFN}			68.074	67.760	21.920	1.00	52.91	E
MOTA	5801	NE2	GIM	E	181	69.329	66.774	23.510	1.00	51.73	E
ATOM	5802	С	GLN	E	181	68.607	65.002	18.277	1.00	45.26	E
MOTA	5803	0	GLN			67.660	64.752	17.530	1.00	46.25	E
ATOM	5804	N	SER			69.448	66.013	18.078		44.33	В
		CA	SER			69.335	66.923	16.943		42.52	E
MOTA	5805										
MOTA	5806	СВ	SER			68.819	68.291	17.401		43.41	E
MOTA	5807	OG	SER			69.658	68.853	18.396		43.07	E
MOTA	5808	C	SER	E	182	70.725	67.068	16.337	1.00	41.70	E
ATOM	5809	0	SER	Е	182	71.726	66.955	17.040	1.00	39.94	E
MOTA	5810	N	PRO	E	183	70.805	67.330	15.023	1.00	41.57	E
MOTA	5811	CD	PRO			69.680	67.554	14.098	1.00	41.72	B
ATOM	5812	CA	PRO			72.087	67.485	14.326		40.68	E
								12.865			E
ATOM	5813	СВ	PRO			71.669	67.638			40.95	
MOTA	5814	CG	PRO		183	70.344	68.309	12.965		42.76	E
ATOM	5815	¢	PRO	E	183	72.988	68.628	14.790		38.81	E
MOTA	5816	0	PRO	E	183	72.520	69.709	15.142	1.00	39.64	B
MOTA	5817	N	ILE	E	184	74.291	68.370	14.785	1.00	37.31	E
MOTA	5818	CA	ILE	E	184	75.270	69.368	15.177	1.00	34.30	E
ATOM	5819	CB	ILE	E	184	76.570	68.728	15.699	1.00	33.43	E
MOTA	5820		ILE			77.671	69.779	15.766		32.87	B
ATOM	5821		ILE			76.337	68.112	17.076		33.53	18
											E
MOTA	5822		ILE			77.530	67.339	17.604		33.29	
MOTA	5823	C			184	75.625	70.216	13.974		33.68	E
MOTA	5824	0	ILE	Е	184	75.851	69.704	12.882		33.87	E
MOTA	5825	N	THR	Ē	185	75.676	71.521	14.181	1.00	34.19	E
MOTA	5826	CA	THR	E	185	76.018	72.431	13.111	1.00	33.39	E
MOTA	5827	CB			185	74.792	73.230	12.637	1.00	33.77	B
MOTA	5828		THR			74.211	73.918	13.751		33.46	E
										33.35	B
ATOM	5829		THR			73.758	72.297	12.016			
MOTA	5830	C			185	77.081	73.396	13.590		33.01	B
MOTA	5831	0	THR	В	185	76.990	73.966	14.679		33.25	E
MOTA	5832	N	VAL	E	186	78.106	73.552	12.770		32.85	E
ATOM	5833	CA	VAL	E	186	79.197	74.453	13.067	1.00	32.84	B
ATOM	5834	СВ			186	80.503	73.684	13.300		31.58	E
ATOM	5835		VAL			81.629	74.651	13.611		30.07	B
ATOM	5836		VAL			80.316	72.697	14.441		30.84	B
						79.329				34.14	B
ATOM	5837	C			186		75.317	11.836			
MOTA	5838	0			186	79.403	74.812	10.719		33.50	E
MOTA	5839	N			187	79.329	76.626	12.029		38.05	E
MOTA	5840	CA	GLU	B	187	79.453	77.522	10.898		40.60	E
ATOM	5841	CB	GLU	В	187	78.35B	78.592	10.934	1.00	43.36	E

ATOM	5842	CG	GLU :	-	107	78.426	79.531	12.121	1.00 47.46	**
								11.886	1.00 47.46	E
MOTA	5843	CD	GLU :		187	77.657	80.822			E
ATOM	5844		GLU			76.452	80.752	11.551	1.00 52.89	B
ATOM	5845		GTA :			78.262	91.908	12.039	1.00 53.48	E
ATOM	5846	C	GLU :			80.819	78.182	10.877	1.00 40.49	B
ATOM	5847	0	GLU			81.496	78.285	11.901	1.00 40.26	E
ATOM	5848	N	TRP		188	81.221	78.610	9.688	1.00 41.52	E
MOTA	5849	CA	TRP	E	188	82.492	79.284	9.488	1.00 43.59	E
ATOM	5850	CB	TRP			83.498	78.337	8.834	1.00 41.24	E
ATOM	5851	CG	TRP	Е	188	84.852	78.942	8.675	1.00 41.34	E
ATOM	5852	CD2	TRP	B	188	85.327	79.672	7.543	1.00 40.23	E
ATOM	5853	CE2	TRP	E	188	86.642	80.090	7.838	1.00 41.87	E
MOTA	5854	CE3	TRP	В	188	84.768	80.015	6.305	1.00 40.90	B
ATOM	5855	CD1	TRP	E	188	85.867	78.945	9.588	1.00 41.88	E
ATOM	5856		TRP			86.947	79.632	9.093	1.00 41.99	B
MOTA	5857		TRP			87.411	80.835	6.938	1.00 42.93	E
ATOM	5858	CZ3	TRP			85.531	80.757	5.408	1.00 42.58	E
ATOM	5859	CH2	TRP		188	86.839	81.159	5.731	1.00 43.65	E
MOTA	5860	C	TRP			82,198	80.467	8.566	1.00 46.04	E
		Ö	TRP			81.335	80.374	7.688	1.00 45.30	B
ATOM	5861								1.00 50.26	E
ATOM	5862	N	ARG			82.899	81.579	8.765		
MOTA	5863	CA	ARG			82.673	82.761	7.936	1.00 54.31	E
ATOM	5864	CB	ARG			81.980	83.855	8.755	1.00 56.19	B
ATOM	5865	CG	ARG			82.820	84.460	9.880	1.00 59.58	B
MOTA	5866	œ	ARG			83.030	83.499	11.045	1.00 63.51	B
ATOM	5867	NE	ARG	B	189	83.580	84.180	12.218	1.00 66.73	B
MOTA	5868	\mathbf{cz}	ARG	E	189	84.771	84.771	12.255	1.00 68.44	B
MOTA	5869	NH1	ARG	E	189	85.553	84.766	11.183	1.00 69.41	E
MOTA	5870	NH2	ARG	E	189	85.178	85.378	13.363	1.00 70.13	E
MOTA	5871	C	ARG	E	189	83.950	83.322	7.313	1.00 55.74	K
ATOM	5872	0	ARG	B	189	85.043	83.182	7.866	1.00 56.16	B
MOTA	5873	N	ALA	E	190	83.796	83.962	6.156	1.00 58.53	E
ATOM	5874	CA	ALA			84.920	84.557	5.435	1,00 60.08	E
ATOM	5875	СВ	ALA			84.550	84.734	3.964	1.00 59.97	E
MOTA	5876	c	ALA			85.335	85.905	6.036	1.00 61.01	B
	5877	Ö	ALA			84.654	86.378	6.971	1.00 62.25	Ē
ATOM						86.338	86.479	5.558	1.00 61.85	E
ATOM	5878	OXT							1.00 32.03	F
MOTA	5879	C	LEU		1	78.718	38.094	33.366		F
MOTA	5880	0	LEU		1	79.818	38.571	33.658	1.00 30.77	
ATOM	5881	N	LEU		1	76.219	38.100	33.307	1.00 33.21	F
MOTA	5882	CA	FEA		1	77.432	38.678	33.953	1.00 32.59	F
MOTA	5883	N	GLN		2	78.578	37.069	32.531	1.00 30.39	F
ATOM	5884	CA	GLN		2	79.744	36.436	31.936	1.00 28.84	P
MOTA	5885	С	GLN	F	2	79.609	36.081	30.462	1.00 27.93	F
MOTA	5886	0	GLN	F	2	78.741	35.308	30.067	1.00 27.68	
MOTA	5887	N	PRO	F	3	80.463	36.663	29.619	1.00 28.02	F
MOTA	5888	CD	PRO	F	3	81.461	37.720	29.856	1.00 28.68	F
ATOM	5889	CA	PRO	F	3	80.370	36.332	28.198	1.00 27.76	P
ATOM	5890	CB	PRO	F	3	81.363	37.298	27.552	1.00 28.01	F
ATOM	5891	CG	PRO	F	3	82.353	37.575	28.660	1.00 28.41	F
ATOM	5892	C	PRO		3	80.774	34.872	28.030	1.00 27.24	P
ATOM	5893	ō	PRO		3	81.698	34,406	28.698	1.00 27.18	
ATOM	5894	N	PHE		4	80.082	34.144	27.159	1.00 25.22	
ATOM	5895	CA	PHE		4	80.409	32.738	26.943	1.00 24.75	
ATOM	5896	CB	PHE		4	79.135	31.905	26.849	1.00 25.85	
	5897	CG	PHE		4	79.272	30.539	27.446	1.00 31.58	
ATOM								28.823	1.00 31.30	
MOTA	5898		PHE		4	79.435	30.384			
MOTA	5899		PHE		4	79.241	29.404	26.639	1.00 32.15	
ATOM	5900		PHE		4	79.561	29.116	29,386	1.00 33.28	
MOTA	5901		PHE		4	79.364	28.136	27.187	1.00 33.29	
ATOM	5902	\mathbf{cz}	PHB		4	79.524	27.989	28.565	1.00 34.18	
ATOM	5903	C	PHE	F	4	81.227	32.588	25.664	1.00 22.43	
MOTA	5904	0	PHE	F	4	80.759	32.919	24.586	1.00 24.59	F
ATOM	5905	N	PRO	F	5	82.460	32.065	25.771	1.00 22.79	
ATOM	5906	æ	PRO	F	5	83.191	31.820	27.029	1.00 21.18	
MOTA	5907	CA	PRO	F	5	83.349	31.882	24.618	1.00 21.18	F
ATOM	5908	СВ	PRO			84.715	32.140	25.218	1.00 20.19	F
ATOM	5909	CG	PRO			84.587		26.544	1.00 20.99	F
MOTA	5910	C	PRO			83.291		23.949	1.00 20.28	F
ATOM	5911	ō	PRO			82.796	29.559	24.521	1.00 19.46	
ATOM	5912	N	GLN			83.818	30.456	22.730	1.00 21.24	
MOTA	5913	CA	GLN			83.848		21.983	1.00 19.98	
MOTA	5914	CB	GLN			83.665		20.484	1.00 18.71	
ATOM	5915	CG	GLN			82.312		20.048	1.00 18.35	
ALON	وبدور	-0		•	•	35.316	20.020			•

3 move	F016	CD.	CT 37	-	_	02 255	20 247	10 500	7 00 00 00	_
ATOM	5916	CD	GLN		6	82.255	30.247	18.537	1.00 22.29	F
MOTA	5917		GLN		6	82.612	29.368	17.740	1.00 21.53	F
MOTA	5918	NB2	GLN	F	6	81.802	31.429	18.138	1.00 20.02	F
ATOM	5919	C	GTM	F	6	85.213	28.548	22.213	1.00 20.47	F
ATOM	5920	0	GFN	F	6	86.243	29.204	22.099	1.00 18.48	F
ATOM	5921	N	PRO	P	7	85.229	27.256	22.575	1.00 21.16	F
ATOM	5922	CD	PRO		7	84.071	26.494	23.084	1.00 20.59	F
ATOM	5923	CA	PRO		7	86.471	26.520	22.813	1.00 21.61	F
ATOM	5924	CB	PRO		7	86.037	25.444	23.797	1.00 23.40	F
MOTA	5925	CG	PRO	F	7	84.649	25.123	23.311	1.00 19.67	F
ATOM	5926	C	PRO	F	7	86.996	25.897	21.521	1.00 23.00	F
MOTA	5927	0	PRO	F	7	86.219	25.601	20.610	1.00 23.19	F
MOTA	5928	N	GLU	F	8	88.312	25.714	21.438	1.00 21.78	F
ATOM	5929	CA	GLŪ		8	88.904	25.068	20.279	1.00 23.12	F
ATOM	5930	СВ	GLU		8	90.297	25.632	19.968	1.00 24.50	F
								18.915		F
MOTA	5931	CG	GTO		8	91.086	24.834		1.00 26.16	
ATOM	5932	CD	GTO		8	90.360	24.697	17.576	1.00 31.57	F
MOTA	5933	OB1	GTA	F	8	89.250	24.114	17.540	1.00 33.65	F
MOTA	5934	OE2	GLU	F	8	90.903	25.171	16.555	1.00 30.66	F
MOTA	5935	C	GLU	F	8	89.005	23.608	20.680	1.00 22.95	F
ATOM	5936	0	GLU	F	8	89.289	23.292	21.833	1.00 23.25	F
ATOM	5937	N	LEU		9	88.756	22.712	19.741	1.00 24.74	F
ATOM	5938	CA	LEU		9	88.815	21.292	20.047	1.00 27.30	F
ATOM	5939	СВ	PEA		9	87.729	20.549	19.272	1.00 25.73	F
ATOM	5940	CG	LEU		9	86.302	21.051	19.494	1.00 29.20	F
MOTA	5941	CD1	LEU	F	9	85.338	20.235	18.645	1.00 28.18	F
MOTA	5942	CD2	LEU	F	9	85.938	20.943	20.967	1.00 29.61	f
ATOM	5943	C	LEU	F	9	90.178	20.707	19.712	1.00 28.17	F
A'TOM	5944	0	LEU		9	90.715	20.940	18.631	1.00 26.94	F
ATOM	5945	N	PRO		10	90.765	19.947	20.647	1.00 30,38	F
ATOM			PRO		10	90.365	19.707	22.044	1.00 30.47	F
	5946	CD CD								
MOTA	5947	CA	PRO		10	92.076	19.355	20.370	1.00 34.24	F
MOTA	5948	CB	PRO		10	92.556	18.915	21.752	1.00 32.97	F
MOTA	5949	CG	PRO	F	10	91.282	18.561	22.448	1.00 31.98	F
ATOM	5950	C	PRO	F	10	91.985	18.188	19.393	1.00 35.94	F
MOTA	5951	0	PRO	F	10	90.993	17.461	19.376	1.00 38.70	F
ATOM	5952	N	TYR		11	93.016	18.031	18.570	1.00 37.40	F
MOTA	5953	CA	TYR		11	93.075	16.936	17.609	1.00 38.84	P
									1.00 38.73	F
ATOM	5954	CB	TYR		11	92.126	17.176	16.434		
ATOM	5955	CG	TYR		11	92.017	15.969	15.539	1.00 39.56	F
MOTA	5956		TYR		11	91.294	14.848	15.942	1.00 39.88	F
MOTA	5957	CE1	TYR	F	11	91.254	13.697	15.164	1.00 39.49	F
ATOM	5958	CD2	TYR	F	11	92.698	15.913	14.327	1.00 39.73	F
MOTA	5959	CE2	TYR	F	11	92.668	14.765	13.537	1.00 40.44	f
ATOM	5960	\mathbf{cz}	TYR		11	91.945	13.659	13.964	1.00 40.29	F
ATOM	5961	ОН	TYR		11	91.921	12.514	13.200	1.00 40.03	F
			TYR			94.498	16.781	17.077	1.00 40.23	F
MOTA	5962	C			11					
ATOM	5963	0	TYR		11	95.102	15.708	17.300	1.00 41.88	P
MOTA	5964	OXT			11	94.988	17.742	16.443	1.00 40.58	F
MOTA	5965	0	HOH	H	1,	37.560	11.197	17.272	1.00 17.47	H
ATOM	5966	0	HOH	H	2	81.295	26.543	20.573	1.00 15.95	H
ATOM	5967	0	HOH	H	3	43.884	23.627	16.726	1.00 14.83	H
MOTA	5968	0	HOH	н	4	89.230	61.015	16.512	1.00 19.10	H
ATOM	5969	Ō	HOH		5	92.090	40.877	18.768	1.00 15.59	н
ATOM	5970	ŏ	HOH		6	57.686	14.054	4.407	1.00 20.02	н
					7	87.607		22.217	1.00 11.29	н
ATOM	5971	0	HOH				31.423			
MOTA	5972	0	HOH		8	31.815	41.479	5.673	1.00 23.91	H
MOTA	5973	0	HOH	H	9	46.112	3.594	18.714	1.00 20.15	H
ATOM	5974	0	HOH	H	10	86.724	67.786	15.551	1.00 22.39	H
MOTA	5975	0	HOH	H	11	42.599	14.833	17.213	1.00 16.12	H
ATOM	5976	0	HOH		12	93.679	37.081	11.737	1.00 15.03	H
ATOM	5977	ō	нон		13	50.288	0.581	25.262	1.00 13.69	H
MOTA			нон		14	96.256	37.853	25.291	1.00 12.90	н
	5978	0							1.00 31.88	н
MOTA	5979	0	нон		15	90.711	30.936	37.307		
ATOM	5980	0	HOH		16	80.045	39.846	25.144	1.00 33.11	H
MOTA	5981	0	HOH		17	80.708	45.662	11.514	1.00 41.56	H
ATOM	5982	0	HOH	H	18	42.215	0.119	11.193	1.00 15.83	H
ATOM	5983	0	HOH	н	19	95,828	50.485	5.930	1.00 27.67	H
MOTA	5984	Ö	HOH		20	48.809	37.278	14.928	1.00 36.10	н.
ATOM	5985	ŏ	нон		21	47.553	-0.403	11.823	1.00 14.62	H
ATOM	5986	Ö	HOH		22	94.554	76.132	19.122	1.00 83.80	н
			HOH		23			17.328	1.00 17.64	H
MOTA	5987	0				83.295	48.460			
MOTA	5988	0	HOH		24	88.976	42.102	7.818	1.00 26.11	H
ATOM	5989	0	HOH	H	25	99.041	56.322	24.823	1.00 24.86	H

MOTA	5990	0	нон н	26	47.640	0.006	20.312	1.00 18.95	H
MOTA	5991	0	нон н	27	46.987	29.359	11.916	1.00 21.84	H
MOTA	5992	0	нон н	28	88.283	37.229	11.279	1.00 21.34	н
MOTA	5993	ō	нон н		49.878	-9.043			
				29			36.424	1.00 32.47	Ħ
MOTA	5994	0	HOH H	30	82.777	39.366	24.935	1.00 24.79	Н,
MOTA	5995	0	нон н	31	72.919	25.704	15.123	1.00 18.09	H
MOTA	5996	0	нон н	32	86.830	25.153	13.558	1.00 24.14	H
ATOM	5997	0	нон н	33	43.152	5.651	13.774	1.00 19.96	н
ATOM	5998	0	нон н	34	100.654	27.732	5.367	1.00 34.73	H
MOTA	5999	0	HOH H	35	48.550	32.122	26.894	1.00 20.17	H
ATOM	6000	0	HOH H	36	78.728	36.578	6.822	1.00 32.92	H
ATOM	6001	0	нон н	37	89.361	11.980	24.953	1.00 51.75	H
MOTA	6002	ō	нон н	38	90.411	24.657	31.926	1.00 28.29	H
ATOM	6003	0	нон н	39	80.690	24.233	8.462	1.00 22.43	H
MOTA	6004	0	нон н	40	83.769	65.973	-5.489	1.00 21.06	H
MOTA	6005	0	HOH H	41	87.710	34.692	7.008	1.00 22.47	H
ATOM	6006	0	нон н	42	38.997	4.521	15.299	1.00 25.36	H
MOTA	6007	ō	нон н	43	94.223	46.644	24.674	1.00 32.67	H
MOTA	6008	0	нон н	44	35.150	15.757	26.294	1.00 29.03	H
MOTA	6009	0	нон н	45	85.059	24.652	18.280	1.00 25.63	H
ATOM	6010	0	нон н	46	67.739	6.320	18.991	1.00 43.67	H
MOTA	6011	0	нон н	47	92.376	63.977	12.866	1.00 32.46	H
MOTA	6012	ō	нон н	48	91.526	49,479	22.504	1.00 29.70	н
ATOM	6013	0	нон н	49	56.333	-2.088	24.733	1.00 28.53	H
ATOM	6014	0	нон н	50	100.482	53.937	3.942	1.00 52.26	H
MOTA	6015	0	нон н	51	48.244	18.753	22.918	1.00 44.88	H
ATOM	6016	o	нон н	52	32.577	-0.558	6.769	1.00 33,70	н
								1.00 29.72	
ATOM	6017	0	нон н	53	47.162	26.527	12.972		Ħ
MOTA	6018	0	HOH H	54	98.621	66.834	5.100	1.00 52.20	H
ATOM	6019	0	нон н	55	88.106	52.134	17.293	1.00 21.13	H
ATOM	6020	0	нон н	56	59.655	31.307	17.069	1.00 25.89	H
ATOM	6021	ō	нон н	57	73.562	24.323	12.997	1.00 23.51	H
						32.725		1.00 52.72	
MOTA	6022	0	нон н	58	43.748		20.165		H
ATOM	6023	0	нон н	59	26.392	-7.072	11.400	1.00 26.20	H
ATOM	6024	0	нон н	60	83.955	73.751	16.805	1.00 18.19	H
ATOM	6025	0	нон н	61	46.229	-19.766	10.675	1.00 28.79	H
ATOM	6026	0	нон н	62	52.436	38.720	16.630	1.00 28.35	H
		ō	нон н	63		9.392		1.00 28.43	н
MOTA	6027				60.555		19.914		
ATOM	6028	0	нон н	64	62.105	2.197	11.948	1.00 33.33	H
ATOM	6029	0	нон н	65	40.514	-12.059	13.631	1.00 21.32	H
MOTA	6030	0	нон н	66	65.876	23.972	14.155	1.00 21.11	H
MOTA	6031	0	нон н	67	84.702	18.013	5.666	1.00 19.12	H
					64.715	11.655	15.936	1.00 28.72	н
ATOM	6032	0	нон н	68					
MOTA	6033	0	нон н	69	85.418	74.949	14.820	1.00 27.90	H
ATOM	6034	0	нон н	70	77.974	25.419	23.038	1.00 42.15	H
ATOM	6035	0	нон н	71	65.805	8.484	20.741	1.00 44.01	н
MOTA	6036	0	нон н	72	51.276	26.045	10.800	1.00 28.36	н
	6037	ō	нон н	73	65.226	22.195	25.831	1.00 36.11	н
MOTA									
ATOM	6038	0	нон н	74	101.567	46.068	1.107	1.00 53.81	H
MOTA	6039	0	нон н	75	32.615	31.234	1.517	1.00 21.03	H
ATOM	6040	0	нон н	76	42.100	-0.001	13.802	1.00 23.44	H
MOTA	6041	0	нон н	77	35,124	40.614	14.668	1.00 27.61	H
MOTA	6042	ō	нон н	78	92.548	46.813	7.595	1.00 31.64	Н
	6043						14.778	1.00 31.04	н
MOTA		0	нон н	79	34.670	13.941			
MOTA	6044	0	нон н	80	98.527	27.671	28.270	1.00 42.07	H
MOTA	6045	0	нон н	81	30.588	36.032	16.540	1.00 37.52	H
MOTA	6046	0	нон н	82	89.345	42.957	13.940	1.00 22.73	H
ATOM	6047	0	нон н	83	92.891	18.085	10.698	1.00 32.35	H
	6048					48.556	16.519	1.00 27.30	н
MOTA		0	нон н	84	90.050				
MOTA	6049	0	HOH H	85	110.812	49.549	15.813	1.00 27.68	H
MOTA	6050	0	нон н	86	75.872	21.668	2.499	1.00 39.37	H
MOTA	6051	0	нон н	87	52.567	14.010	7.270	1.00 34.20	H
MOTA	6052	ō	нон н	88	69.016	32.569	12.651	1.00 36.96	H
MOTA	6053	Ö			96.637	25.945	31.742	1.00 37.26	H
			нон н	89					
MOTA	6054	0	нон н	90		-12.998	8.560	1.00 22.82	H
MOTA	6055	0	нон н	91	113.021	48.469	17.945	1.00 47.59	H
ATOM	6056	0	нон н	92	34.266	25.052	23.930	1.00 31.02	H
MOTA	6057	0	нон н	93	51.464	31.946	19.300	1.00 15.75	H
MOTA	6058	ō	нон н	94	80.054	50.912	15.041	1.00 25.94	H
							16.393		н
MOTA	6059	0	нон н	95		-13.432		1.00 39.73	
MOTA	6060	0	нон н	96	57.701		7.708	1.00 25.27	H
MOTA	6061	0	нон н	97	80.838	52.853	26.436	1.00 27.67	H
MOTA	6062	0	нон н	98	58.205	13.023	20.294	1.00 27.57	H
ATOM	6063	ō	нон н	99	41.832		15.601	1.00 27.32	н
		•		-		551251			

MOTA	6064	o	HOH H 100	72.807	29.880	11.618	1.00 28.05	н
ATOM	6065	ō	HOH H 101	48.499	5.079	4.053	1.00 38,72	H
MOTA	6066	ō	нон н 102	100.679	66.408	9.019	1.00 36.21	H
MOTA	6067	ŏ	HOH H 103	45.023	41.442	11.747	1.00 42.72	H
ATOM	6068	ŏ	HOH H 104	83.296	63.483	-2.738	1.00 27.46	н
MOTA	6069	ō	HOH H 105	85.067	29.522	34.732	1.00 35.62	н
ATOM	6070	ŏ	HOH H 106	72.272	53.390	15.314	1.00 38.75	H
MOTA	6071	ŏ	HOH H 107	80.600	27.688	5.225	1.00 26.04	
ATOM	6072	Ö	HOH H 108	71.251	18.567			H
ATOM	6073	ŏ	HOH H 109	88.274	65.356	16.503	1.00 29.08	H
ATOM	6074	0	HOH H 110	43.031		19.510	1.00 26.70	H
MOTA	6075	o	HOH H 111	101.304	4.836 35.384	7.813	1.00 38.59	H
MOTA	6076	o	HOH H 112	44.554	10.725	4.755 19.619	1.00 43.53	H
MOTA	6077	ŏ	HOH H 113				1.00 21.38	H
MOTA	6078	ŏ	HOH H 114	115.506	34.478	5.615	1.00 46.62	H
MOTA	6079	Ö	HOH H 115		-25.634	9.802	1.00 42.69	H
MOTA	6080	Ö	HOH H 116	38.663	-33.304	20.170 -2.715	1.00 61.12	H
MOTA	6081	ŏ	HOH H 117		26.161		1.00 31.39	H
MOTA	6082			105.197	41.384	18.739	1.00 38.53	H
MOTA	6083	0	HOH H 118 HOH H 119		-12.372	18.422	1.00 32.47	H
ATOM	6084			45.430	15.732	9.556	1.00 32.39	н
		0	HOH H 120	70.475	9.817	-1.029	1.00 53.38	H
MOTA	6085	0	HOH H 121	87.895	64.540	22.445	1.00 47.01	H
MOTA	6086	0	HOH H 122	39.337	36.650	16.644	1.00 25.21	H
ATOM	6087	0	HOH H 123	104.091	50.783	20.204	1.00 31.31	H
MOTA	6088	0	HOH H 124	72.528	13.825	20.909	1.00 62.81	H
MOTA	6089	0	HOH H 125	55.353	-5.411	5.747	1.00 25.46	H
MOTA	6090	0	HOH H 126	97.848	63.704	25.177	1.00 27.84	H
MOTA	6091	0	HOH H 127	89.799	75.117	14.074	1.00 49.56	H
MOTA	6092	0	HOH H 128	96.226	35.565	0.211	1.00 40.25	н
MOTA	6093	0	HOH H 129		-15.445	19.161	1.00 37.04	H
MOTA	6094	0	нон н 130	90.627	52.974	9.649	1.00 22.70	H
ATOM	6095	0	HOH H 131	114.398	29.773	11.425	1.00 42.36	н
MOTA	6096	0	нон н 132	69.810	89.608	-0.164	1.00 53.48	H
MOTA	6097	0	нон н 133	99.069	30.421	4.728	1.00 31.21	H
MOTA	6098	0	HOH H 134	37.335	49.129	5.746	1.00 43.90	H
ATOM	6099	0	HOH H 135	77.753	73.821	17.600	1.00 50.43	H
MOTA	6100	0	нон н 136	44.853		11.090	1.00 21.26	Н
MOTA	6101	0	HOH H 137	88.697	80.608	-4.574	1.00 49.42	H
ATOM	6102	0	HOH H 138	62.018	-6.136	9.010	1.00 30.19	H
MOTA	6103	0	нон н 139	35.964	-5.810	5.494	1.00 45.47	H
MOTA	6104	0	HOH H 140	73.968	65.480	8.013	1.00 43.93	H
MOTA	6105	0	HOH H 141	78.361	66.868	24.455	1.00 57.76	H
MOTA	6106	0	HOH H 142	53.527	3.199	22.332	1.00 32.95	H
MOTA	6107	0	HOH H 143	56.018	-6.530	25.205	1.00 42.75	H
MOTA	6108	0	HOH H 144	82.930	52.617	28.345	1.00 32.35	H
MOTA	6109	0	HOH H 145		-21.313	24.210	1.00 48.87	H
MOTA	6110	0	HOH H 146	86.079	41.197	35.698	1.00 36.97	H
MOTA	6111	0	HOH H 147	35.017	8.399	11.516	1.00 32.21	H
MOTA	6112	0	HOH H 148		-19.905	17.166	1.00 41.53	H
MOTA	6113	0	HOH H 149	55.504	20.659	6.959	1.00 36.63	н
MOTA	6114	0	HOH H 150	106.046	47.260	19.571	1.00 30.60	H
MOTA	6115	0	HOH H 151	108.769	26.147	5.447	1.00 48.82	н
MOTA	6116	0	HOH H 152	38.689	17.576	4.331	1.00 39.07	H
MOTA	6117	0	HOH H 153	97.787	62.580	8.740	1.00 29.61	H
ATOM	6118	0	HOH H 154		-12.817	20.769	1.00 50.36	H
MOTA	6119	0	нон н 155	47.887	40.072	-4.641	1.00 51.05	H
MOTA	6120	0	нон н 156	60.057	16.564	27.477	1.00 40.66	H
ATOM	6121	0	нон н 157	67.048	27.841	20.873	1.00 39.66	н
MOTA	6122	0	нон н 158	37.028	32.932	18.669	1.00 37.23	H
MOTA	6123	0	HOH H 159	121.780	18.693	-3.076	1.00 46.64	н
MOTA	6124	0	HOH H 160	39.196	18.091	27.271	1.00 29.99	H
MOTA	6125	0	HOH H 161	113.285	44.237	19.561	1.00 39.04	H
MOTA	6126	0	HOH H 162	43.379	27.754	19.370	1.00 27.58	H
MOTA	6127	0	HOH H 163	91.636	66.903	11.885	1.00 54.73	H
MOTA	6128	0	HOH H 164	113.381	46.844	20.020	1.00 54.22	H
MOTA	6129	0	HOH H 165	79.238	62.082	24.112	1.00 36.07	H
MOTA	6130	0	нон и 166	27.985	32.355	18.424	1.00 36.25	H
MOTA	6131	0	HOH H 167		-10.661	20.615	1.00 9.89	H
MOTA	6132	0	нон н 168	93.577	37.339	20.182	1.00 14.03	H
MOTA	6133	0	нон н 169	97.912	51.662	7.309	1.00 24.22	H
MOTA	6134	0	HOH H 170	69.616	4.375	18.521	1.00 38.01	H
MOTA	6135	0	HOH H 171	80.870	25.194	6.002	1.00 21.84	H
MOTA	6136	0	HOH H 172	50.564	12.887	5.906	1.00 32.25	H
MOTA	6137	0	нон н 173	88.207	37.288	13.919	1.00 19.68	H

ATOM	6138	0	HOH H 174	93.800	47.651	27.174	1.00 41.65	н
ATOM	6139	0	HOH H 175	52.842	0.304	25.210	1.00 28.07	н
MOTA	6140	0	нон н 176	66.457	4.742	14.051	1.00 28.64	H
MOTA	6141	0	HOH H 177	36.948	12.416	15.109	1.00 28.66	H
MOTA	6142	0	HOH H 178	103.292	41.793	7.607	1.00 28.51	H
ATOM	6143	0	HOH H 179	86.476	36.035	9.339	1.00 27.43	H
MOTA	6144	0	HOH H 180	82.262	41.159	26.845	1.00 24.13	H
ATOM ATOM	6145 6146	0	HOH H 181 HOH H 182	32.348 69.916	15.030	26.400	1.00 30.06	H
ATOM	6147	ŏ	HOH H 183	48.060	30.709 10.142	14.482 26.751	1.00 42.81 1.00 49.12	H
ATOM	6148	ō	HOH H 184	45.863	-9.131	37.252	1.00 43.70	H
ATOM	6149	ō	HOH H 185	32.095	-3.806	34.251	1.00 41.46	н
MOTA	6150	Ō	нон н 186	108.258	31.975	8.914	1.00 33.62	н
ATOM	6151	0	нон н 187	99.465	64.293	8.210	1.00 54.43	H
MOTA	6152	0	нон н 188	74.677	30.785	27.841	1.00 28.20	H
MOTA	6153	0	нон н 189	44.953	0.968	35.892	1.00 32.25	H
MOTA	6154	0	нон н 190	88.523	27.792	36.268	1.00 30.83	H
ATOM	6155	0	HOH H 191	37.736	8.611	11.729	1.00 38.92	H
MOTA	6156	0	нон н 192	35.988	45.178	12.964	1.00 33.85	H
ATOM	6157	0	HOH H 193	77.222	68.027	1.401	1.00 27.02	H
MOTA MOTA	6158 6159	0	НОН Н 194 НОН Н 195	63.326 109.635	-8.764 61.489	15.926 27.644	1.00 38.46 1.00 52.79	H
ATOM	6160	Ö	HOH H 196	101.299	67.528	11.319	1.00 38.92	H H
ATOM	6161	ō	нон н 197	77.295	56.116	25.768	1.00 36.83	H
ATOM	6162	ŏ	нон н 198	81.538	22.288	0.320	1.00 47.08	н
ATOM	6163	Ō	нон н 199	55.989	3.900	0.756	1.00 46.35	H
ATOM	6164	0	нон н 200	66.200	40.514	17.513	1.00 43.54	н
ATOM	6165	0	HOH H 201	40.497	-1.046	9.238	1.00 27.84	H
ATOM	6166	0	HOH H 202	57.171	27.504	8.258	1.00 52.74	H
ATOM	6167	0	нон н 203	44.592	-6.430	37.531	1.00 37.55	H
ATOM	6168	0	нон н 204	26.892	-1.642	9.494	1.00 55.58	H
MOTA	6169	0	нон н 205	83.350	58.389	2.759	1.00 46.24	H
ATOM ATOM	6170 6171	0	НОН Н 206 НОН Н 207	112.353 86.315	45.284 23.927	9.770 16.100	1.00 30.99 1.00 41.36	H H
ATOM	6172	o	HOH H 208	67.053	45.396	12.396	1.00 31.02	н
ATOM	6173	ŏ	нон н 200	111.609	60.418	8.362	1.00 52.01	H
ATOM	6174	ō	HOH H 210	91.254	47.553	32.752	1.00 41.71	H
MOTA	6175	0	нон н 211	88.489	39.944	11.117	1.00 34.00	H
ATOM	6176	o	HOH H 212	104.972	69.233	16.415	1.00 37.26	H
ATOM	6177	0	нон н 213	23.462	39.893	6.692	1.00 56.45	H
MOTA	6178	0	HOH H 214	84.114	54.447	-1.718	1.00 42.58	H
ATOM	6179	0	HOH H 215	105.045	66.068	22.775	1.00 24.48	H
ATOM	6180	0	HOH H 216	85.378	52.388	17.025	1.00 37.91	H
MOTA MOTA	6181 6182	0	HOH H 217 HOH H 218	91.411 99.019	30.837 37.803	4.259 25.178	1.00 23.59 1.00 37.20	H
ATOM	6183	ŏ	HOH H 219	88.866	41.183	35.781	1.00 42.88	H
MOTA	6184	ō	нон н 220	66.946	25.931	12.530	1.00 45.53	н
ATOM	6185	ō	HOH H 221	83.809	61.544	-0.645	1.00 32.51	н
MOTA	6186	0	нон н 222	91.766	28.386	3.286	1.00 29.97	H
MOTA	6187	0	HOH H 223	83.302	45.674	11.423	1.00 40.65	H
ATOM	6188	0	HOH H 224	59.198	3.628	18.904	1.00 22.61	H
MOTA	6189	0	HOH H 225		-11.852	5.930	1.00 29.77	H
MOTA	6190	0	HOH H 226	88.953	22.712	24.560	1.00 23.54	H
ATOM	6191	0	HOH H 227	108.379	54.102	21.160	1.00 30.79	H
ATOM ATOM	6192 6193	0	НОН Н 228 НОН Н 229	44.957 105.872	16.820 50.217	6.827 22.393	1.00 37.14 1.00 33.77	н
MOTA	6194	ŏ	HOH H 230	40.390	52.287	-1.729	1.00 62.00	н
ATOM	6195	ö	HOH H 231	103.837	27.586	24.806	1.00 50.76	H
ATOM	6196	ō	HOH H 232	50.931	9.397	25.207	1.00 40.65	H
ATOM	6197	0	HOH H 233	64.739	2.382	27.973	1.00 46.98	H
MOTA	6198	0	нон н 234	38.363	0.460	8.402	1.00 28.58	H
MOTA	6199	0	нон н 235	73.577	50.129	18.561	1.00 36.68	H
MOTA	6200	0	нон н 236	100.912	58.519	6.876	1.00 36.99	H
MOTA	6201	0	нон н 237	100.664	26.841	26.380	1.00 36.27	H
MOTA	6202	0	HOH H 238	82.528	48.080	12.484	1.00 44.97	H
ATOM	6203	0	HOH H 239	70.870	44.782 -9.049	13.746	1.00 26.53 1.00 59.29	H H
ATOM ATOM	6204 6205	0	HOH H 240 HOH H 241	71.914 28.024	9.146	17.302 32.377	1.00 59.29	H
ATOM	6205	0	HOH H 242	55.531	-2.470	4.880	1.00 50.20	н
ATOM	6207	ŏ	HOH H 243	63.362	16.623	21.334	1.00 30.95	H
ATOM	6208	ō	HOH H 244	71.813	27.548	12.914	1.00 54.77	H
MOTA	6209	0	HOH H 245	22.793	-3.930	12.731	1.00 39.10	H
ATOM	6210	0	HOH H 246	73.087	44.091	34.124	1.00 47.86	H
MOTA	6211	0	HOH H 247	48.717	31.774	19.850	1.00 33.46	H

MOTA	6212	0	HOH H 248	100.851	61.218	7.741	1.00 35.49	H
MOTA	6213	0	HOH H 249	116.291	47.311	12.227	1.00 49.67	н
MOTA	6214	0	HOH H 250	99.469	40.748	22.418	1.00 25.82	H
ATOM	6215	0	HOH H 251	52.271	4.031	24.614	1.00 44.68	H
MOTA	6216	0	HOH H 252	106.629	40.298	32.271	1.00 59.44	H
MOTA	6217	0	нон н 253	45.587	-9.303	3.049	1.00 26.81	H
MOTA	6218	0	HOH H 254	52.547	-9.432	27.670	1.00 45.08	H
MOTA	6219	0	нон н 255	75.854	21.157	27.640	1.00 42.33	H
MOTA	6220	0	нон н 256	82.119	63.444	23.430	1.00 37.84	H
MOTA	6221	0	HOH H 257	104.091	38.660	18.936	1.00 30.29	H
ATOM	6222	0	нон н 258	79.477	56.121	8.190	1.00 39,16	H
MOTA	6223	0	HOH H 259	101.351	32.257	5.631	1.00 29.94	H
MOTA	6224	0	HOH H 260	93.989	23.313	31.488	1.00 35.30	H
MOTA	6225	0	HOH H 261	28.754	-1.723	6.977	1.00 36.90	H
MOTA	6226	0	HOH H 262	93.007	48.370	9.901	1.00 49.06	H
MOTA	6227	0	HOH H 263	82.990	88.137	9.529	1.00 39.70	H
ATOM	6228	0	HOH H 264	118.031	51.582	0.542	1.00 36.21	H
ATOM	6229	0	нон н 265	21.682	15.046	11.602	1.00 62.29	H
MOTA	6230	0	HOH H 266	34.210	24.576	5.314	1.00 18.89	H
ATOM	6231	0	HOH H 267	85.829	40.095	14.911	1.00 25.26	н
ATOM	6232	0	HOH H 268	102.070	38.308	21.059	1.00 41.79	H
MOTA	6233	0	HOH H 269	41.071	-2.346	7.039	1.00 38.87	H
MOTA	6234	0	HOH H 270	68.717	3.686	16.083	1.00 37.79	H
MOTA	6235	0	нон н 271		-12.649	12.753	1.00 29.26	H
MOTA	6236	0	HOH H 272	36.426	24.744	4.145	1.00 45.88	H
ATOM	6237	0	HOH H 273	88.670	31.858	5.525	1.00 39.43	H
ATOM	6238	0	HOH H 274	90.819	38.524	36.028	1.00 30.15	H
ATOM	6239	0	HOH H 275	90.790	49.861	10.317	1.00 39.97	H
ATOM	6240	0	HOH H 276	77.026	11.969	13.970	1.00 44.87	н
MOTA	6241	0	HOH H 277	36.555	12.078	12.344	1.00 40.47	H
ATOM	6242	0	HOH H 278	52.331	7.302	24.972	1.00 49.30	H
MOTA	6243	0	нон н 279	92.612	33.229	3.564	1.00 40.55	H
ATOM	6244	0	HOH H 280	83.546	64.142	25.612	1.00 50.28	H
ATOM	6245	0	HOH H 281	28.206	-1.891	36.868	1.00 44.06	H
MOTA	6246	0	HOH H 282	93.185	20.914	30.917	1.00 44.51	H
ATOM	6247	0	HOH H 283	98.176	41.763	24.500	1.00 44.20	H
ATOM	6248	0	HOH H 284	29.174	-0.123	4.304	1.00 46.75	H
MOTA	6249	0	HOH H 285	79.206	77.643	14.919	1.00 30.21	H
ATOM		ō	нон н 286			37.436	1.00 36.96	H
	6250			90.531	26.085			
ATOM	6251	0	HOH H 287	55.726	0.396	21.054	1.00 49.55	H
MOTA	6252	0	HOH H 288	111.246	30.915	19.699	1.00 42.91	H
ATOM	6253	ō	HOH H 289	77.000	58.921	5.300	1.00 47.04	н
ATOM	6254	Ο,	HOH H 290	34.339	-9.458	5.288	1.00 25.50	H
MOTA	6255	0	HOH H 291	109.784	29.168	15.534	1.00 45.96	H
ATOM	6256	0	HOH H 292	93.674	48.853	29.650	1.00 48.76	н
ATOM	6257	0	нон н 293	92.299	47.066	3.801	1.00 37.41	H
MOTA	6258	0	HOH H 294	110.965	23.141	11.799	1.00 42.97	H
ATOM	6259	0	HOH H 295	90.562	45.235	33.919	1.00 33.83	H
ATOM	6260	0	HOH H 296		-10.500	25.018	1.00 49.78	H
MOTA	6261	0	HOH H 297	54.676	36.195	11.362	1.00 54.22	H
MOTA	6262	0	HOH H 298	107.263	59.234	5.282	1.00 56.05	H
MOTA	6263	ō	нон н 299	70.560	48.918	1.476	1.00 49.72	H
		-						
· ATOM	6264	0	нон н 300	84.037	38.916	5.971	1.00 39.33	H
MOTA	6265	0	HOH H 301	86.468	41.381	11.971	1.00 45.69	H
ATOM	6266	o	HOH H 302	24.400	11.569	23.610	1.00 36.73	H
MOTA	6267	0	HOH H 303	73.087	79.808	7.028	1.00 46.20	H
ATOM	6268	0	HOH H 304	72.681	43.116	14.941	1.00 51.84	H
ATOM	6269	0	нон н 305	84.844	42.198	15.611	1.00 26.23	H
ATOM	6270	0	нон н 306	54.135	19.007	24.978	1.00 27.41	H
ATOM	6271	0	нон н 307	67.044	10.459	18.465	1.00 44.92	H
MOTA	6272	0	нон н 308	82.262	49.436	14.864	1.00 39.04	H
MOTA	6273	0	нон н 309	114.093	50.994	16.895	1.00 43.32	H
MOTA	6274	0	HOH H 310	64.428	3.092	30.590	1.00 43.29	H
MOTA	6275	ō	HOH H 311	81.152	70.187	18.656	1.00 34.21	н
MOTA	6276	0	нон н 312	74.596	81.584	-2.515	1.00 55.00	H
MOTA	6277	0	нон н 313	61.161	25.774	22.464	1.00 32.98	H
ATOM	6278	0	HOH H 314	53.149	-7.019	4.754	1.00 26.01	н
MOTA	6279	0	HOH H 315	44.571	8.317	33.567	1.00 40.32	H
MOTA	6280	0	нон н 316	82.293	49.769	10.587	1.00 35.22	H
ATOM	6281	0	HOH H 317	48.467	8.859	24.614	1.00 42.38	н
ATOM	6282	0	нон н 318	56.588	-8.027	4.728	1.00 44.65	H
MOTA	6283	0	HOH H 319	31,280	-23.239	26.551	1.00 42.45	H
ATOM	6284	0	нон н 320	82.483	40.137	7.719	1.00 39.22	н
				82.063	19.937	23.440	1.00 35.69	н
ATOM	6285	0	HOH H 321					

MOTA 6286 a HOH H 322 106.025 63.366 22.616 1.00 31.93 H MOTA 6287 ٥ HOH H 323 46.181 9.890 8.669 1.00 38.11 H MOTA 6288 HOH H 324 71.708 75.568 6.998 1.00 41.82 H ATOM 6289 0 HOH H 325 108.280 34.405 3.851 1.00 30.72 H ATOM 6290 O HOH H 326 32.275 40.921 14.635 1.00 40.72 H ATOM 6291 0 HOH H 327 37.556 15.785 5.690 1.00 42.29 H MOTA 6292 0 HOH H 328 85.569 33.598 37.182 1.00 31.78 н ٥ 33.070 -11.287 23.137 ATOM 6293 HOH H 329 1.00 48.90 н MOTA 6294 0 HOH H 330 87.593 16.513 19.683 1.00 45.53 H MOTA 6295 0 HOH H 331 116.176 53.631 17.853 1.00 39.81 H 6296 0 HOH H 332 26.940 -11.377 14.930 H MOTA 1.00 39.40 ATOM 6297 O HOH H 333 60.033 28.679 22.456 1.00 32.84 н MOTA 6298 0 HOH H 334 52.472 15.182 2.562 1.00 48.72 н ATOM 6299 0 HOH H 335 84.377 54.588 4.646 1.00 40.99 н н 0 HOH H 336 115.759 19.970 ATOM 6300 67.454 1.00 46.15 MOTA 6301 0 HOH H 337 88.969 52.684 25.112 1.00 42.31 H ATOM 6302 O HOH H 338 36.351 12.852 9.875 1.00 37.11 6303 0 нон н 339 97.702 31.578 2.653 1.00 49.82 H MOTA 53.964 HOH H 340 -6.543 26.981 1.00 35.52 Н MOTA 6304 0 17.094 ATOM 6305 0 HOH H 341 24.475 -17.438 1.00 38.04 H ATOM 6306 HOH H 342 58.530 0.915 19.036 1.00 43.08 H 1.00 48.54 6307 0 HOH H 343 77.156 37.203 39.025 MOTA 0.435 Н HOH H 344 49.978 -1.361 1.00 39.48 ATOM 6308 0 MOTA 6309 0 HOH H 345 53.900 37.104 13.703 1.00 47.74 H MOTA 6310 O HOH H 346 77.886 49.625 13.575 1.00 57.13 8.721 0.570 Н 57.053 1.00 50.38 0 HOH H 347 ATOM 6311 MOTA 6312 0 HOH H 348 96.803 63.745 10.854 1.00 41.14 Н 89.009 70.808 11.906 1.00 45.67 Н ATOM 6313 HOH H 349 6314 ٥ HOH H 350 66.363 22.353 8.221 1.00 42.47 Н ATOM 6315 52.578 25.044 8.541 1.00 41.16 H ATOM 0 HOH H 351 MOTA 6316 0 HOH H 352 81.789 73.640 ~3.536 1.00 50.48 н 0 67.632 -11.181 13.891 1.00 48.24 н MOTA 6317 HOH H 353 6318 0 HOH H 354 41.357 -5.652 22.367 1.00 14.47 ATOM -5.096 30.876 1.00 23.96 G MOTA 6319 C1 EDO G 501 37.685 38.224 1.00 23.38 G MOTA 6320 01 EDO G 501 -4.213 31.883 MOTA 6321 C2 EDO G 501 38.742 -6.046 30.406 1.00 25.29 G G MOTA 6322 02 EDO G 501 39.062 -6.931 31.464 1.00 26.30 MOTA 6323 Cl EDO G 502 89.146 26.377 27.000 1.00 41.69 G 26.508 28.343 1.00 51.10 ATOM 6324 01 **EDO G 502** 88.631 EDO G 502 88.436 25.261 26.303 1.00 43.14 G ATOM 6325 C2 MOTA 6326 02 EDO G 502 88.726 24.052 26.967 1.00 41.73 EDO G 503 85.093 31.920 30.633 1.00 21.00 G C1 ATOM 6327 G 31,203 1.00 18.65 MOTA 6328 01 EDO G 503 85.283 30.597 6329 EDO G 503 83.846 32.561 31.186 1.00 19.69 MOTA C2 ATOM 6330 02 EDO G 503 84.148 33.101 32.454 1.00 20.94 G 34.956 3.907 25.885 1.00 38.01 EDO G 504 6331 C1 ATOM G 33.976 2.838 25.869 1.00 36.69 ATOM 6332 01 EDO G 504 MOTA 6333 C2 EDO G 504 36.360 3.344 25.982 1.00 39.84 G 02 EDO G 504 36.573 2.396 24.935 1.00 33.51 ATOM 6334 END

Example 4

Binding of altered gluten peptides (peptide analogs) to MHC molecules is assayedwith purified HLA molecules. Binding of labeled peptide to purified HLA DQ2 molecules can be measured as described by Johansen et al. (1996) Int Immmunol (8), 177-82. Briefly, purified DQ2 molecules (50 - 1000 nM) are incubated with the 125-I radiolabeled indicator peptide (MB 65kDa 243-255Y, sequence KPLLIIAEDVEGEY; 20 000 cpm, 1-5 nM) at pH 4.9. After incubation for 24 hours, the peptide bound to DQ2 and the non-bound peptide are separated on Sephadex G25 superfine spun columns. The radioactivity in the bound and non-bound fractions was counted in a gamma-counter, and the fraction of peptide bound to DQ2 (cpm in the bound fraction/total cpm recovered) is calculated. The binding capacities of the peptide binding inhibitors are assayed by testing their ability to inhibit the binding of the labeled indicator peptide. The concentration required to give 50%

inhibition (IC $_{50}$) is calculated. Since the level of IC $_{50}$ may vary between separate titration experiments, the IC $_{50}$ values are compared to the IC $_{50}$ of a reference peptide by determining the relative binding capacity (RBC), which is the ratio: IC $_{50}$ of reference peptide / IC $_{50}$ of test compound. HLA-DQ2 molecules can be isolated by antibody affinity chromatography from lysates of HLA-DQ2 homozygous Epstein Barr virus transformed B-lymphoblastoid cell lines (detergent solubilized) or from water soluble, recombinant molecules produced similarly as described in Example 3 above. The recombinant molecules can be made with or without covalently linked peptide and with a biotin recognition sequence at the C-terminal end of the β -subunit that facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling alternative ways for measurement of IC $_{50}$. A peptide analog with an IC $_{50}$ value of less than 100 μ M is suitable for further screenings.

[92] Alternatively, binding of altered gluten peptides to HLA-DQ2 can also be assayed using the soluble DQ2 heterodimer produced as described in Example 3 above. The presence of the biotin recognition sequence at the C-terminal end of the β-subunit facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling measurement of IC₅₀ or K_I.

Candidate peptide analogs are further tested for their ability to inhibit proliferation of [93] T cells specific for gluten peptides. This is done by using HLA-DQ2 restricted T cell clones (TCC) and glutaraldehyde fixed antigen presenting cells (e.g. Epstein Barr virus transformed B-lymphoid transformed cells) expressing HLA-DQ2. The antigen presenting cells are pelleted and resuspended in RPMI containing 0.05% glutaraldehyde for 90 sec, whereafter glycin to a final concentration of 0.2 M is added for 60 sec. The cells are then washed, counted, and resuspended in PBS or PBS buffered with citrate phosphate to a final pH of 4.9. The fixed APC are incubated overnight with various concentrations of peptides. The inhibitory peptides are usually added 30 min prior to the stimulatory peptide. The antigen presenting cells are then washed twice and resuspended in culture medium of RPMI-1640 supplemented with 15% v/v heat inactivated pooled human serum and the T cells are added. The experiments are performed in triplicates of 3-5 X 10⁴ TCC with 5 X 10⁴ fixed APC and various titrations of inhibitory and stimulatory peptides. Following an incubation period of 48 hours, each culture is pulsed with [3H]-thymidine for an additional 12-18 hours. Cultures are then harvested on fiberglass filters and counted as above. Mean CPM and standard error of the mean are calculated from data determined in triplicate cultures. Peptide analogs that inhibit proliferation to approximately 25% at a concentration of 50 µM or greater are suitable for further screening.

[94] All publications and patent applications cited in this specification are herein incorporated by reference as if each individual publication or patent application were specifically and individually indicated to be incorporated by reference.

[95] Although the foregoing invention has been described in some detail by way of illustration and example for purposes of clarity of understanding, it will be readily apparent to those of ordinary skill in the art in light of the teachings of this invention that certain changes and modifications may be made thereto without departing from the spirit or scope of the appended claims.

WHAT IS CLAIMED IS:

1. An HLA-binding peptide inhibitor; wherein said inhibitor is an analog of an immunogenic gluten oligopeptide of at least about 8 residues in length, wherein the immunogenic gluten oligopeptide is altered by the replacement of one or more amino acids; and wherein said analog binds tightly to HLA molecules; is proteolytically stable; and does not activate disease-specific T cells.

- The HLA-binding peptide inhibitor of Claim 1, wherein said analog comprises
 one or more naturally occurring amino acids, non-naturally occurring amino acids, modified
 amino acids, or amino acid mimetics.
- 3. The HLA-binding peptide inhibitor of Claim 2, wherein said analog is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.
- 4. The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises at least one PXP motif.
- 5. The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises a sequence selected from the group consisting of: PQPELPY; PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ; PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PYPQPELPY and PYPQPQLPY.
- [96] 6. The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence PXPQPELPY, where X is Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp or Glu.
 - 7. The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.
 - 8. The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.
 - 9. The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence $PFPQX_1ELX_2Y$, where X_1 and X_2 are independently selected from 4-hydroxy-Pro, 4-amino-Pro, or 3-hydroxy-Pro, and proline, with the proviso that at least one of X_1 and X_2 is a residue other than proline

10. The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.

- 11. The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.
- 12. A method of treating Celiac Sprue and/or dermatitis herpetiformis, the method comprising:

administering to a patient an effective dose of an HLA-binding peptide inhibitor; wherein said HLA-binding peptide inhibitor attenuates gluten toxicity in said patient.

- 13. The method of Claim 12, wherein said HLA-binding peptide inhibitor is administered with a glutenase.
- 14. The method according to Claim 12, wherein said HLA-binding peptide inhibitor is administered orally.
- 15. The method according to Claim 12, wherein said HLA-binding peptide inhibitor is contained in a formulation that comprises an enteric coating.
- 16. A formulation for use in treatment of Celiac Sprue and/or dermatitis herpetiformis, comprising:

an effective dose of an HLA-binding peptide inhibitor and a pharmaceutically acceptable excipient.

- 17. The formulation according to Claim 16, further comprising an enteric coating.
- 18. Use of an HLA-binding peptide inhibitor in the treatment of HLA-DQ2 positive individuals who are either pre-disposed to type I diabetes or have developed symptoms of type I diabetes.
- 19. A computer for producing a three-dimensional representation of a molecule wherein said molecule comprises an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, wherein said computer comprises:
- a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic

gluten oligopeptide;

a working memory for storing instructions for processing said machine-readable data;

- a central-processing unit coupled to said working memory and to said machinereadable data storage medium for processing said machine readable data into said threedimensional representation; and
- a display coupled to said central-processing unit for displaying said three-dimensional representation.
- 20. A computer-assisted method for identifying potential modulators of Celiac Sprue and/or dermatitis herpetiformis, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
- (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, thereby generating a criteria data set;
- (b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;
- (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;
- (d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.